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One goal of the research initiative is to foster both the correct commercial code development and its proper use for the benefit of research and technological development. The objectives are to: define the problem of software code verification and validation, define the problem of precision testing for software code verification and validation, establish guidelines for reliable and safe numerical Simulations, develop standards for numerical simulations, and define qualifications and requirements for FE/FD-Code users. These objectives may hold in general, but in order to restricted time and money we will first focus on a well defined class of problems: Contact Detonations and Impact/Penetration Problems. This is a first necessary step towards the final goal of an international standard.

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Contact Detonations
and Impact/Penetration Problems:

Demonstration of a Procedure to Establish Guidelines for Reliable and Safe Numerical Simulations

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Preface

In year 2002, at the *World Conference on Computational Mechanics (WCCM)* in Vienna, there will be a key topic for the first time: *"Verification and Validation in Computational Mechanics"* (V&V). Besides one main session about "Reliability and Safety", there are two minisymposia about V&V organized. An accademic V&V-minisymposium is organized by Professor N.-E. Wiberg (Europe) and an industrial one is organized by Dr. L. Schwer (USA). We are participating in the latter one.

This final report - **Demonstration of a Procedure to Establish Guidelines for Reliable and Safe Numerical Simulations** - presented here, is our contribution of a cowork on V&V. It has been conducted by the European Office of Aerospace Research and Development, US Air Force Research Laboratory, US Air Force Office of Scientific Research.

The contractual partners are the University of the Bundeswehr Munich in Germany - Dept of Civil Engineering - Professor N. Gebbeken and the U.S.A. - US Air Force Research Office. The contractual processing time has been from June 1^{st} 2000 to May 31^{st} 2001, and the deadline of this final report is July 14^{th} 2001.

Our work has to be understood as a *discussion proposal.* Our focus of interest in V&V is certainly not terminated by this work. Review and comments are most welcome, and this report is free for discussion now. Therefore, we are also looking forward to an interesting and lively discussion at the *WCCM* next year.

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Chapter 1

Motivation

1.1 Introduction

Numerical analysis is not only the domain of experts. Low cost computing power and a wide range of commercial analysis tools are readily available. Tools such as CAD geometry transfer, automatic meshing, adaptive refinement and optimization devices means that products have become much easier to use.

This has led to many analyses being carried out throughout the entire product design cycle and to the rapid use of analysis technologies by smaller companies (NAFEMS [27]).

Not only companies, but also scientific institutions are tending to reduce costly and time consuming experiments and to rely more and more on the results of numerical simulations in order to reduce the time and the amount of money needed for research and development. Unfortunately, institutions often have not the education needed for proper use of these techniques. Numerical methods are - methodical inherent - approximate methods, and therefore they are open for misuse and the production of any possible error. Subsequently, model validation is necessarily required. Indeed, the cost benefit analysis has become predominant in the field of research & development in engineering, in natural science, etc. .

There is a considerable concern that the *accuracy* of numerical simulations using finite methods is required to be *verified* in order to allow the results to be effectively *evaluated.* "Accuracy", "verification", "evaluation", (and other terms) are terms to be well defined (section 1.3).

1.2 Objective

The objective of this study is the **demonstration of a procedure to establish guidelines for reliable and safe numerical simulations**. Therefore, reliable numerical studies of engineering

tasks have to be established and the credible use of finite methods as well as the ensurance of their accuracy has to be promoted.

Main fields of investigation

Doing this, three main fields of investigation have to be addressed:

1. Theories of finite methods,
2. numerical tools and
3. the user.

Key questions

Therefore, three key questions have to be approached:

1. What are the limitations of the **theories of finite methods** used?
2. What are **the numerical tools** able to solve?
3. What abilities are required from **the user**?

The main fields have to be discussed with respect to four levels:

- Evaluation,
- Validation,
- Accreditation, and
- Quality assurance,

in order to guarantee the quality of finite methods, software and user, and their proper interaction. These terms will be defined in the following in section 1.3.

Focus

Because the entire field of finite methods and numerical simulations is so broad we focus in this research program on **penetration and contact explosion problems**.

Nevertheless, there are

- general statements, valid in any case, and
- specific statements, only valid for the problem studied and the used software package.

1.3 Provision of a standard

One intention of our investigations presented here is to provide the basics for **the reliability of numerical simulations**, in order to develop a kind of *standard.*

Herein, specific key terms will be well defined. Such are, for example:

- Errors and user mistakes (section 1.3.2.3)
- Model simplifications (section 2.2)
- Code validation and verification (section 3.3)

By this *standard* at hand, the user will be able to evaluate his results, to detect and estimate errors on each level of modeling and ultimately to improve his numerical calculations concerning their reliability. The user is accompanied by a **guideline** during all necessary steps of his analysis that is transferable for his specific tasks.

The following definitions are primarily taken from DIN EN ISO 9000:2000-12 ("quality management systems: fundamentals and vocabulary") [14]. Some definitions are modified here with respect to our specific subject of interest.

1.3.1 Scope of application

Quality management (QM) and quality assurance are also relevant here. Specific principles and key terms have been well defined in the standard DIN EN ISO 9000 that has been accepted by the European committee for standardization (CEN) as an European standard in December 2000.

The basic key terms will be defined in the section below.

The origins of the ISO 9000 family are - among others - related to military standards. The first ISO (International Standard Organisation) - standards for quality assurance are based on various national quality standards of the 80'ies and 90'ies; especially: The Canadian standards "Z 299", the British standard "BS 5750-quality assurance", the US military NATO standard "AQAP" and the German "DIN" standards.

DIN EN ISO 9000 includes the basics of QM and is the first part of the ISO 9000 family of standards that has been developed to assist organizations, of all types and sizes, to implement and operate effective quality management systems.

This standard is applicable to the following:

1. *organizations seeking advantage through the implementation of a QM system,*
2. **organizations seeking confidence** *from their suppliers that their product requirements will be satisfied,*
3. **users of the products,**
4. *those concerned with a mutual understanding of the terminology used in quality management,*
5. *those internal or external to the organization who assess the QM system or audit it for conformity with the requirements if ISO 9001 (e.g. auditors, regulators, certification/registration bodies),*
6. *those internal or external to the organization who give advice or training on the QM system appropriate to that organization,*
7. **developers of related standards.**

No. 2., 3. and 7. are especially of interest here, and thus, we are motivated to go further into detail.

1.3.2 Basic key terms

1.3.2.1 General terms related to quality

requirement
Need or expectation that is stated, generally implied or obligatory.

quality
Degree to which a set of inherent characteristics fulfills requirements.

capability

Ability of an organization or process to realize a product that will fulfill the requirements for that product.

quality assurance

Part of quality management (QM) focused on providing confidence that quality requirements will be fulfilled.

quality characteristic

Inherent 'distinguishing feature' (=characteristic) of a product or process related to a requirement.

continual (quality) improvement

Increasing the ability to fulfill quality requirements as a recurring activity.

effectivenes

Extent to which planned activities are realized and planned results achieved.

efficiency

Relationship between the result achieved and the resources used.

interested party

Person or group having an interest in the performance or success of an organization.

process

Set of in interrelated or interacting activities which transforms inputs into outputs.

product

Result of a process. There are four generic product categories: services, software, hardware, processed materials.

dependability

Collective term used to describe the availability performance and its influencing factors: reliabil-

ity performance, maintainability performance, and maintenance support performance. Dependability is used for general desciptions only and it is not quantifiable.

traceability and transparency
Ability to trace the history, application or location of that which is under consideration.

robustness
The question of robustness about a product is a criterion for the sensitivity of the process: How do specific (but minor) modifications within the process influence the resulting product? *(own definition).*

conformity and accuracy
Conformity is the fulfillment of a requirement. In our subject, the accuracy of numerical results is a key requirement that has to be fulfilled. ("Non-conformity" and related terms will be defined below.)

1.3.2.2 Terms related to examinations

inspection and testing
Inspection is a conformity evaluation by observation and judgement accompanied as appropriate by measurement, testing or gauging.

verification
Confirmation, through the provision of objective evidence (data supporting the existence or verity of something), that specified requirements have been fulfilled.

validation
Confirmation, through the provision of objective evidence (s. verification), that the requirements of a specified intended use or application have been fulfilled.

qualification process
Process to demonstrate the ability to fulfill specified requirements. Qualification can concern persons, products or systems.

review

Activity undertaken to determine the suitability, adequacy and effectiveness of the subject matter to achieve established objectives. Example: Nonconformity review.

audit

Systematic, independent and documented process for obtaining audit evidence and evaluating it objectively to determine the extent to which (specific) audit criteria are fulfilled. Internal audits, sometimes called "first-party audits", are conducted by, or on behalf of, the organization itself for internal purposes and can form the basis for an organization's self-declaration of conformity. External audits include what are generally termed "second-" or "third-party audits". Second-party audits are conducted by parties having an interest in the organization, such as customers, or by other persons on their behalf. Third-party audits are conducted by external independent organizations. Such organizations provide certification or registration of conformity with specific requirements.

1.3.2.3 Specific terms related on non-conformity and others

At this point we would like to point out that we have to distinguish between error, mistake, and other terms related to this topic.

Definitions:

non-conformity

Non-fulfillment of a requirement.

defect

Non-fulfillment of a requirement related to an intended or specified use.

preventive action

Action to eliminate the cause of a potential nonconformity or other undesirable potential situation.

corrective action

Action to eliminate the cause of a detected nonconformity or other undesirable situation.

correction

Action to eliminate a detected non-conformity.

error

Error is a deviation from the ideal. And an error can be methodical inherent. All finite methods produce errors. Therefore, a research field has been established that deals with 'error detection', 'error estimation' and 'error minimization'.

mistake

Mistake is "doing wrong". A mistake is something that must be avoided.
Such mistakes are, for example:

- Wrong use or a misestimation of specific methods,
- misapplication of software,
- misinterpretation of numerical results,
- misinterpretation of errors(!).

1.3.3 About "Accreditation, Certification and Quality Assurance"

The following is an example of an general idea. It is cited from the Accreditation, Certification and Quality Assurance Institute [ACQuIn, WOLFF, Universität Bayreuth, 95440 Bayreuth]:

Accreditation is an evaluation based on agreed standards, resulting in a formal, public recognition of a programme (or an institution). It is a democratic, transparent process resting upon self- and peer-assessment for improvement of academic quality and public accountability. There are two complementary procedures: first an evaluation procedure consisting of the self evaluation of the applicant plus the on-site inspection and the report of the evaluator group, followed by the accreditation procedure in which the relevant expert team analyses and discusses the self report and the evaluators' recommendation, before the accreditation commission decides on accreditation, conditional accreditation subject to provisos or conditions, or denial of accreditation.

1.3.4 Principles of quality management concerning our objective

Success can result from implementing and maintaining a management system that is designed to continually improve performance while adressing the needs of all interested parties [14].

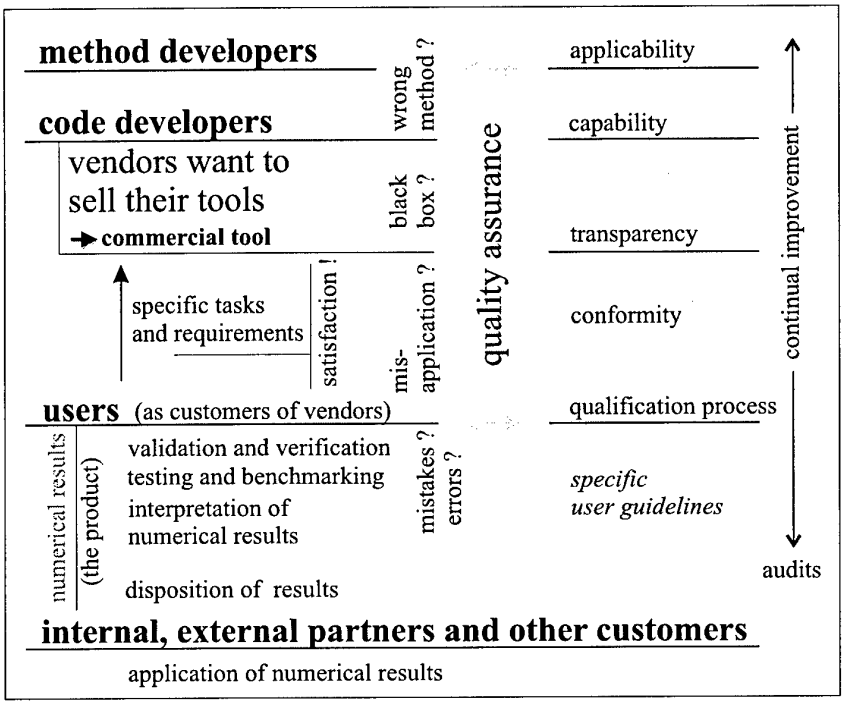


Figure 1.1: Interested parties and quality assurance

As fig. 1.1 shows, the interested parties (here) are:

- method and code developers
- tools' vendors
- users who dispose numerical results
- internal and external partners (e.g. testing institutes)
- persons/customers who apply the results

Of course, all parties have specific interests and requirements that might differ from each other. But their proper interaction is crucial for an efficient quality assurance.

The user, for example, has got a legitimate requirement that the promisses of the code vendors, who primarily want to sell their products, are fulfilled. Those who apply numerical results have

certain interest that the results - e.g. presented and disposed by the user - are reliable and safe or validated and verified. But, up to now, the only one responsible for the numerical result is the user!

Some of the quality management principles identified in the standard are basically also relevant here:

1. customer focus
2. involvement of people
3. system approach to management
4. continual improvement
5. factual approach to decision making

1.) **Customer focus**: *Organizations depend on their customers and therefore should understand current and future customer needs, should meet customer requirements and strive to exceed customer expectations.*

It is a principal part of QM to focus on the customer. Here we have to focus on the person/organization who wants to apply results of numerical simulations to his/its specific technical problem. Therefore, the reliablility of results is a main interest. Thus, customer orientation is also important here for all parties mentioned above, especially for code vendors.

Considered the code vendor and the code user as contractual partners, customer requirements have to be defined and satisfied (fig. 1.1). The user requires tools with characteristics that satisfy his needs and expectations. This needs and expectations are expressed in product specifications and collectively referred to as customer requirements. "The reliable and safe numerical simulation of high velocity impact and perforation in the range of 100 - 1000 $\frac{m}{s}$ impact velocity, 1-100 g (metal-) penetrator weight into a (unreinforced) mortar kind of material" may be specified conctractually by the customer (= user) or may be determined by the organization (tool's vendor) itself. In either case, the customer ultimately determines the acceptability of the product.

Annotation: Considered the code user and the persons who apply results as contractual partners, this concept can be transfered respectively.

2.) **Involvement of people**: *People at all levels are the essence of an organization and their full involvement enables their abilities to be used for the organization's benefit.*

This principle can be transfered to our task when education, experience and competency is taken into account of all people involved. In this context, special focus on user requirements has to be done. But also the proper interaction of people (experts, developers, users, ...) comes within the limits of this topic: Safe and relible numerical simulations are - at least - the result of teamwork based on the proper involvement of all parties.

3.) **System approach to management**: *Identifying, understanding and managing interrelated processes as a system contributes to the organization's effectiveness and efficiency in achieving its objectives.*

Transfered to our task, the intention of this principle is to understand the numerical simulation as a **process**. The desired result (reliable numerical simulations) is achieved more efficiently when **activities** (method development, programming, implementation of numerical features and models into the code, numerical setup and calculation, ..., interpretation of results, technical application, research and further development, ...) and related **recources** (monetary environment and input, development time, deployment and personnel qualification ← user requirements, ...) are managed as a **process within a system**. Therefore the partners have not only to be treated as contractual partners, as described in no.#1 and the term "organization" may be 'ascended' to a higher level: It should include the whole system of all parties and their (proper!?) interactions.

4.) **Continual improvement**: *Continual improvement of the organization's overall performance should be a permanent objective of the organization.*

Beyond the aim to improove method, tools and users a QM system has got the aim of continual improvement of itself by increasing the probability of enhancing the satisfaction of customers and other interested parties. Analysing and evaluating the existing situation is a first action for improvement that has to be transfered also to our topic.

A goal of QM here, is the continual improvement of performance of methods, codes and tools. Therefore, the responsible persons of this three key levels have to separately review and assure quality continuously. The method has to be scrutinized, codes have to be verified and user requirements have to be defined and accredited. Audits on each level have to be done independently.

Feedback from 'customers' (see above) and other interested parties, audits and review of the QM system can also be used to identify opportunities for (continual) improvement.

5.) **Factual approach to decision making**: *Effective decisions are based on the analysis of data and information.*

To heed this principle is important to act on the maxim of quality assurance: The factual approach must be fundament of the evaluation of methods, codes and users.

In this context, the importance of a documentation of the entire process has to be mentioned: *Documentation enables communication of intent and consistence of action:*

- achievement of conformity to stated requirements,
- provision of appropriate user training,
- repeatability, traceability and objective evidence of numerical results,
- evaluation of the effectiveness and continuing suitability of the QM system.

For the purpose of this definition, documentation is a value-adding activity in terms of a continual quality improvement.

Again, all levels have to be embraced: A documentation of the method yields insight in the theoretical background. The documentation of codes prevents 'black boxes'. The documentation of numerical studies detailed by the user is an instrument of self control and contributes to repeatability of results.

And, besides the regard to each level for its own, the association of the levels is important, too: Therefore, essentially the following types of documents are used in QM systems:

- *quality manuals* that provide consistent information about the organization's QM system;
- *quality plans* that describe how the QM system is applied to a specific product (code);
- *specifications* that state requirements;
- *guidelines or work instructions* that state recommendations or suggestions or that provide information about how to perform activities and processes consistently;
- *(and others)*

In general: The extent of documentation depends on factors such as the type and size of organization, the complexity and interaction of processes, the complexity of products, customer requirements, the applicable regulatory requirements, the demonstrated ability of personnel,

and the extent to which it is necessary to demonstrate fulfillment of quality management system requirements.

Transfered to our specific topic, main focus should be done on the regard to each level for its own. We are going further into detail; see below.

1.3.5 Conclusion

Generally:

Section 1.3 has outlined quality aspects and quality key terms (section 1.3.2), generally and with special focus on our subject.

Without going deeper into the details of standards like the mentioned DIN EN ISO 9000 family, we asserted that a proper quality management is also necessary for reliability and safety of numerical simulations. Again, we would like to point out the importance of a proper interaction of *all interested parties* (section 1.3.4, fig. 1.1).

Our special focus here:

This report establishes a guideline for the user to detect and evaluate errors on each level of the numerical analysis.
→ **Error**s must be detected and minimized.

The proposal, presented here, might also to be understood as a trainee program or a **qualification process** related to **quality assurance** for numerical calculations with special respect to hyper dynamics.
→ **Mistake**s will be reduced by following these proposals.

The user is educated by that way and might be **accredit**ed as an expert of specific numerical methods. Therefore a test - possibly as a part of internal or/and external **audit**s - might be included in the future.

Risks are unfolded and a deep insight into the method or the code used is established, and this allows to see behind the curtain. The intention is a **continual improvement** of methods, codes and users regarding their **quality**.

1.4 Classifications

The following is mainly related to the specific problem of penetration and contact detonation. In order to select the proper methodology we need to define and classify the problem precisely with respect to load, structure, material and the goal of investigation.

1.4.1 Static case, structural dynamics and hyper dynamics

First of all, we need to distinguish between time effects where mass forces are generated (dynamic case) and where mass forces are not generated (static case). Furthermore, the dynamic case has to be subdivided into hyper dynamics and ordinary dynamics - i.e. structural dynamics. This has to be taken into account when using numerical methods:

- **Static case**: Analytical or 'hand'- calculations are in some cases possible and often sufficient to solve simple static problems or they can (roughly) verify numerical calculations; linear/nonlinear - ordinary - FEM calculations are still necessary and challenging for large and/or irregular geometric problems; material models are known for most instances; reference tests and benchmarks are broadly available. The numerical methods and the codes used are overall known.
- **Structural dynamics**: A reference to the static case is oftentimes possible (e.g. by enhancement factors); which finite method is best, depends on the task to be solved (see section 2.3.5). The numerical methods and the codes used are state of the art.
- **Hyper dynamics**: Analytical calculations are not available and 'hand' formulas - if available - are normally confined to specific empirical studies; to obtain material data is often a difficult task. The numerical methods are specialized (e.g. wave propagation codes / hydrocodes) and some further error possibilities are - methodical inherent - introduced (as shown below in chapter 3). Therefore, primarily in hyper dynamics, code validation & verification, reference tests and benchmarks are principal duties in order to obtain reliable numerical results.

For the sake of a classification of *dynamic* and *hyper dynamic* effects on structures, different load types and important values as impact duration, impact velocity, strain rate, ratio of dynamic to static strength, material behavior and related testing device are compared in table 1.1.

Table 1.1 is based on data from different publications that have been collected and complemented here (e.g. BISCHOFF & PERRY (1995) [6], ZUKAS (1982) [36]).

Table 1.1: Comparison of important key values, taken (and modified) from GEBBEKEN & RUPPERT [21]

loadings	impact duration $\approx \mu s$	impact velocity in m/s	strain rate locally $\dot{\epsilon}$ in $1/s$	f_c^{dyn}/f_c^{stat} pressure	f_c^{dyn}/f_c^{stat} tension	material behavior	testing device
–	$> 10^{11}$	–	$< 10^{-6}$	1.0	1.0	creep & shrinkage	hydraulic
traffic	$> 10^7$	–	$< 10^{-6}$	1.0	1.1	elastic (el)	hydrodyn. pneumatic
wind (gust)	$> 10^7$	< 60	$< 10^{-4}$	1-1.2	1.5	visc.-el	wind test
earth quake	10^7	–	$10^{-3} - 10^0$	1-1.3	1.8	visc.-el-pl	dynamic
water waves	10^6	< 5	$10^{-3} - 10^{-1}$	1-1.3	1.7	visc.-el	wave tests
debris impact	10^6	< 10	$< 10^1$	1-2.0	2.3	el-pl	hammer test
plane crash	10^5	< 90	$10^{-2} - 10^2$	1-1.3	2.5	el-pl-dam	"
impact	10^4	< 30	$10^{-2} - 10^2$	1-1.3	2.5	el-pl-dam	"
blast wave	10^3	< 4000	$10^1 - 10^3$	1-2.0	5	el-pl-dam dam = damage	split hopkinson pressure bar flyer-plate-
conventional weapon			10^2	1.5-2.0	?	damage	&
			10^3	3	?		edge-on- impact
contact expl.	10^1	< 9000	$< 10^8$	> 3	?	hydr-pl-dam	explosion
comet impact	10^1	> 12000	$< 10^8$	?	?	vaporizes	gas gun

Loadings are mostly not of static nature. In fig. 1.2, different load types and time dependent phenomena are related to measured strain rates in concrete. In addition, the increase of the compressive strength with increasing strain rates is shown up to the limit of $10^2 \frac{1}{s}$. There is still a lack of data beyond that limit.

Not mentioning when strain rates are greater than $10^2 \frac{1}{s}$ is not *reliable*; it is not an *error*, it is a *mistake*, or at least 'wantonly negligent'.

In fig. 1.3, tension stress vs. strain is shown for two different strain rates. These curves are valid for reinforcing steel BSt420/500, DIN1045 (German standard for reinforced concrete structures), with a deterministic yield limit of $\sigma_{yield} = 420\text{MPa}$. The higher the rate, the more stress can be taken.

Figures 1.2 and 1.3 are two examples that show typical material behavior due to different loading situations and strain rates. What is shown here for concrete and a specific reinforcing steel from DIN1045, is generally valid for other materials, too.

For highly dynamic loads we also refer to G. R. JOHNSON's publication [25] where data for metals up to $\dot{\epsilon} = 10^3 \frac{1}{s}$ are presented.

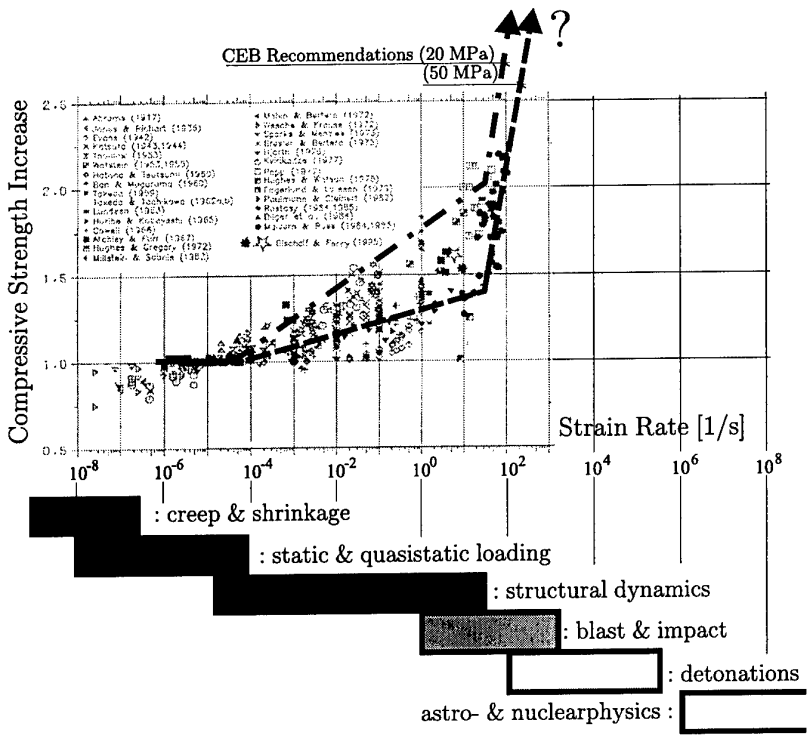


Figure 1.2: Compressive strength versus strain rate, $f_c(\dot{\epsilon})$, and related phenomena (based on BISCHOFF & PERRY [6])

The behavior of materials and structures subjected to static or quasistatic loads, as well as creep & shrinkage phenomena have been investigated in the past decades. Structural dynamics ($\dot{\epsilon} < 10^2 \frac{1}{s}$) is well known from the methodical point of view, but is still challenging when applying new materials or damping devices, respectively. There is a lot of literature available to solve such conventional problems.

Most of the material parameters are actually rate dependent. There are two ways to take rate dependency into account:

1. rheological modeling,

2. multiply the static values by an amplification factor.

The latter is a common strategy and will also be applied here. The amplification factor f_c^{dyn}/f_c (Table 1.1) can be obtained only by testing. We have taken the values of the amplification factor from the trilinear regression curve suggested by the CEB-BULLETIN NO.187(1987), [8] - [11] as shown for concrete in fig. 1.2.

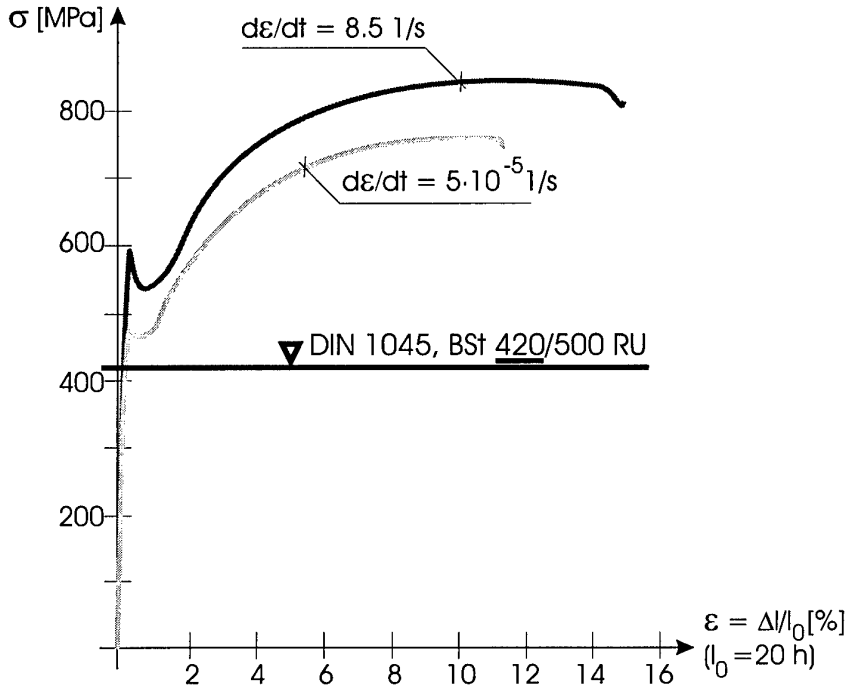


Figure 1.3: Stress vs. strain, reinforcing steel from DIN1045

Conclusion

Different loading situations (tab. 1.1) cause different material and structural behavior that require different numerical methods to be used.

An extrapolation from structural dynamics to hyper dynamics is often not the appropriate way (fig. 1.2), because of both lack of data and different material and structural behavior.

In the following section, we focus on hyper dynamics.

1.4.2 Levels of material modeling in continuum mechanics

Before going into details of material modeling in hyper dynamics, one should be aware of the different levels of material models that might be possible.

It depends on the problem to be solved, which level is the most appropriate one. In order to model real structures, often the homogenization hypothesis is adopted which enables the formulation of the constitutive equations on the level of macromechanics (fig. 1.4).

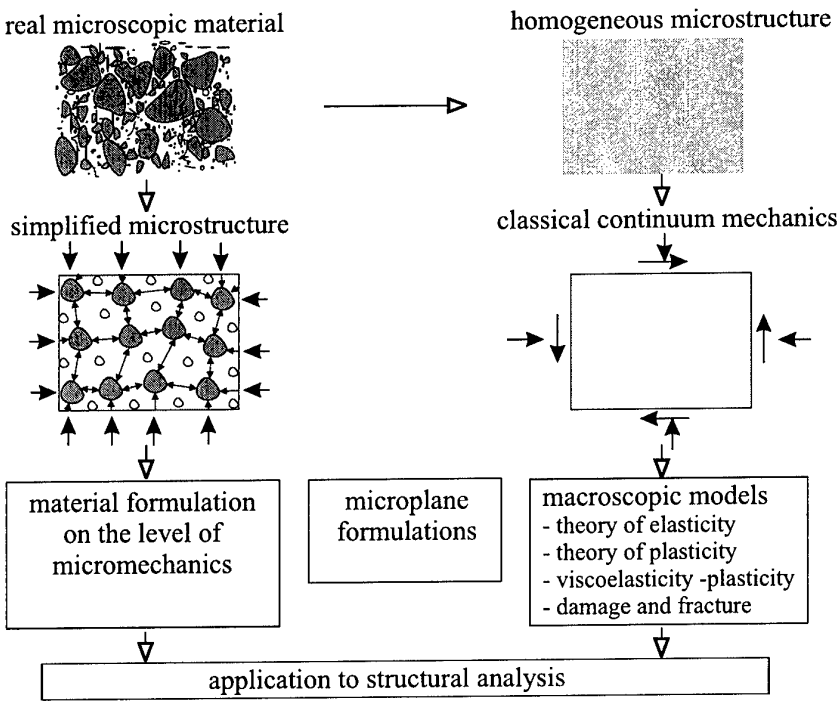


Figure 1.4: Homogenization of a microscopic material to a macroscopic scale (RUPPERT & GEBBEKEN [31], [22])

Annotation

Adopting the homogenization assumption we must realize, that the information of the individual constituents is smeared out (homogenised). Although concrete, for example, is a highly inhomogenious material, this is commonly done when modeling on the macroscopic scale.

Micromechanic approximations are very time consuming, what sometimes is unacceptable; especially for huge problem setups.

1.4.3 Structural behavior

Structural behavior is influenced by many factors including the distribution of loads, the duration at which loads are applied, interaction with adjacent structural components, the material properties, the stiffness of individual members and devices and stiffness of overall structure, mass distribution, temperature influence, etc. . All of these aspects comprise specific idealizations (simplifications) to some ideal form representing the **reality**.

Whether the impact causes mostly local (fig. 1.5(a)) and/or global effects (fig. 1.5(b,c)), is

essentially based on peak pressure, impact duration and area, and the proportion between the masses of impactor and target.

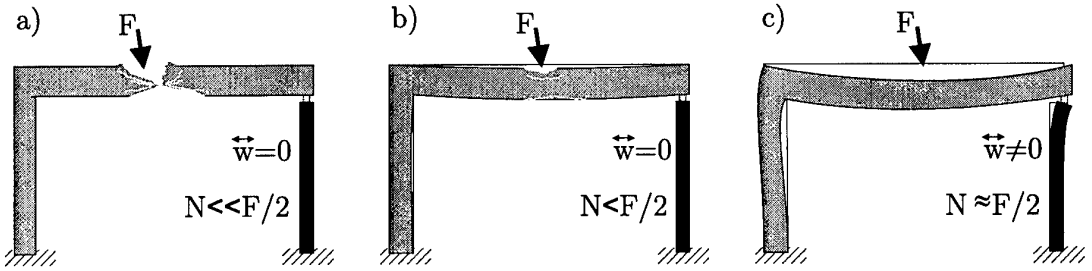


Figure 1.5: Frame, structural response: a) hyper dynamics, b) dynamics, c) quasi statics

An impact duration within milli- or microseconds is related to hyper dynamics. The global structural response is within some Hertz; this means some oscillations per second. Therefore, it becomes evident that the structure is often too inert to react in total as a whole structure under hyper dynamic actions (fig. 1.5(a)). This is demonstrated by an impactor with a relative small mass penetrating the structure by high velocity impact. The heavy structure is much too inert to react in total. No observable displacement occurs (w=0) and almost no response forces are generated (N<<F/2).

In case b) and c), the impact velocity is less than in case a) and/or the impactor is heavier. Thus, in addition to local damage also global structural response occurs and reaction forces in the system are generated. In case a) and b) special finite methods have to be used, e.g. hydrocodes (chapter 3). In case c) a classical-method-based calculation in the range of structural dynamics (e.g. BIGGS [5], EIBL [16]) may be sufficient.

1.4.4 Consequences

Section 1.4 has shown significant variations in material as well as in structural responses caused by different load situations. Different engineering tasks ask for different numerical methods and different software tools. In the next section, specific methods are generally and briefly presented.

The more challenging the task investigated, the more fundamental knowledge of physics and methods used is required. Therefore an introduction into finite methods will be presented.

Chapter 2

Finite methods - Relevant basics

2.1 Introduction

Nowadays, one cannot imagine any numerical calculation in the fields of applied mechanics without using finite methods. Finite methods (FM) means finite element methods (FEM) and finite difference methods (FDM). The boundary element method (BEM) and the family of meshless methods (Smoothed Particle Hydrodynamics, Element-Free Galerkin, ...) will not be discussed here.

Numerical methods allow us to replace a set of differential equations by a set of linearized equations. The finite methods are generally procedures for approximating the set of differential equations. Numerical methods are used because they allow approximate solutions of a broad range of problems which otherwise could not be solved. Problems with irregular boundaries, sophisticated material models, geometrical nonlinearities and difficult boundary conditions, for example, are unsolvable analytically. Furthermore, optimization strategies, extensive parameter studies, etc. are impossible without numerical studies.

The growing use of powerful hardware enables the implementation of more complicated and larger systems into the numerical code (software). As computing power became more widely available, industry increasingly started to solve practical engineering problems using finite methods in order to ensure quality and to reduce time needed for development.

2.2 About Modeling

2.2.1 Basic remarks

Before one executes a numerical simulation by using finite method codes, a mechanical model which represents the reality has to be implemented into the code by numerical modeling.

In general, the different steps of modeling are roughly as follows:
Reality → simplifications → **Mechanical model** → simplifications → **Numerical model.**

Although computer resources now permit models of high complexity to be processed, in most analyses there remains a requirement to simplify the problem to be solved. Simplifications are necessary "engineering approaches".

Every model is an abstraction and simplification of the reality, and, therefore, incorporates model-inherent errors; deviations from the reality.

The degree of simplification depends on both, the accuracy required and the resources available. Thus, when the idealized structure is analysed, by finite element methods for example, deviations from the real structure will certainly arise depending on the assumptions made.

The following basic remarks are taken (and modified) from REDDY et al. [29].

Modeling is an art, based on the ability to "visualize" the physical reality. All basic and applied knowledge of physical problems, finite elements, and solution algorithms contributes to modeling expertise.

In (numerical) modeling, the principal difficulty faced by a typical user of a code is to understand the physical action and boundary conditions of the actual structure, and the limitations of applicable theory, well enough to prepare a satisfactory model. Another difficulty is to understand the behaviors of various elements, and the tool's options or code's limitations, well enough to make an intelligent choice among them. The result may be a poor specification of the problem to be solved, a model that fails to reflect important features of the physical problem, fine detail irrelevant to the problem, a solution based on inappropriate loading or support conditions, and a surplus of computed results which are not properly examined and questioned (I.C. Taig: "Finite Element Analysis in Industry - Expertise or Profiency?", 1984).

Numerical modeling is more than just laying out a mesh.

2.2.2 The way in general

Fig. 2.1 - taken (and modified) from K.-J. BATHE "Finite-Elemente-Methoden" [2] - summarizes the process of finite method analysis and it shows the way in general.

The finite method will solve only the model selected. All assumptions made for this model will be reflected therefore. Hence, the choice of an appropriate mechanical model - or some specific models - is a key step, and the solution of the mechanical model is only one part of the process of analysis.

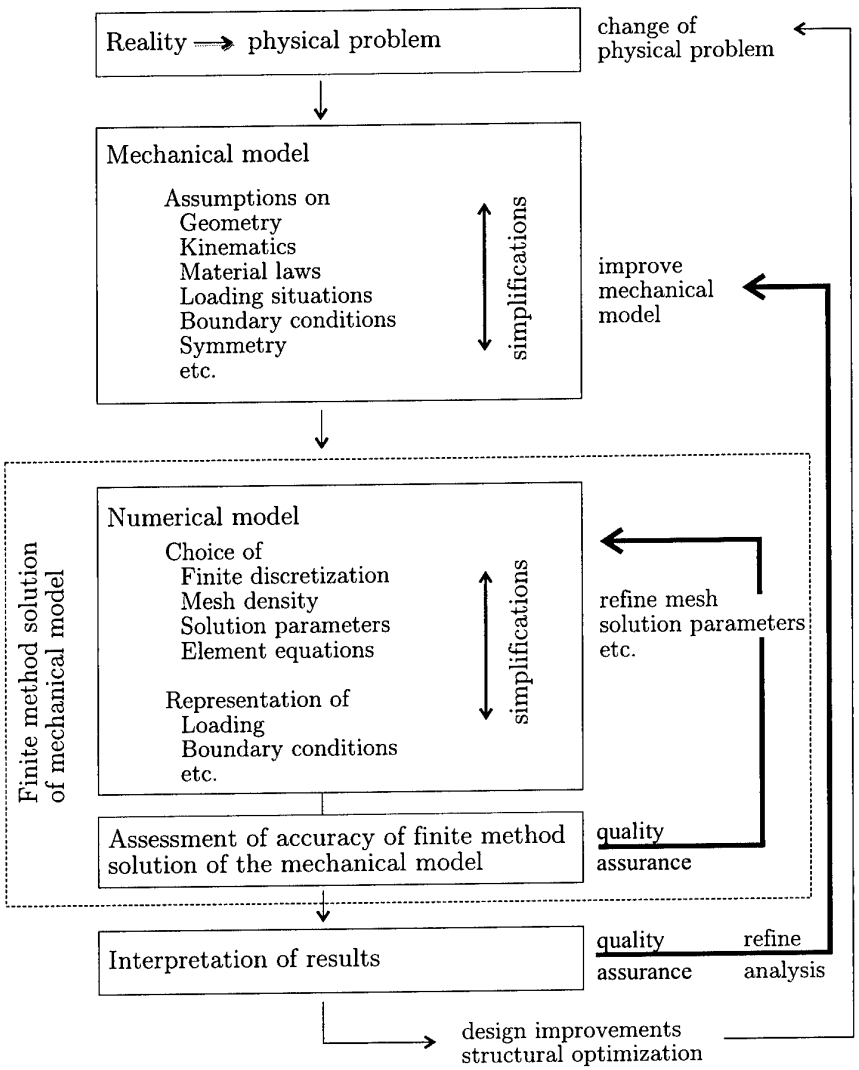


Figure 2.1: The way of finite method analysis in general; taken (and modified) from BATHE [2]

2.2.3 Introductory examples

The way described before was a general way of the process of analysis. Nevertheless, one should carefully specify the scheme shown in fig. 2.1. The authors, e.g., have specified the scheme with respect to contact detonation problems in [32], that is abstracted in section 2.2.3.3.

2.2.3.1 Mechanical modeling - example: Structural engineering - steel frame

First of all, some pre-work has to be done in order to find the proper mechanical model. Such can be, for example, hand calculations, previous analysis on smaller and easier models and physical tests. Doing so, a careful appraisal of FE results gives more insight into model behavior.

A physical task might be, for example, to design a steel frame construction. The actual structure is shown in fig. 2.2. Fig. 2.3 illustrates specific mechanical models of the given problem of fig. 2.2 as given on a shop-drawing.

Indeed, this task is understood as a fundamental engineering job, but already up to this point inevitable *errors* (here: deviations from reality) occur, because an exact and unequivocal description of reality does not exist. That is why fig. 2.3 illustrates only a choice of some feasible mechanical idealizations that are typically used in the field of engineering mechanics and structural engineering. A basic lecture at the university on structural engineering might contain these illustrations.

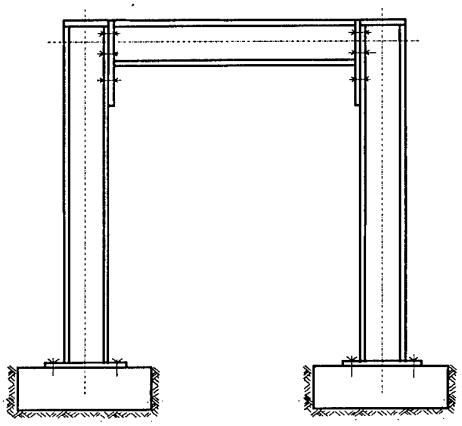


Figure 2.2: Example: Real frame structure

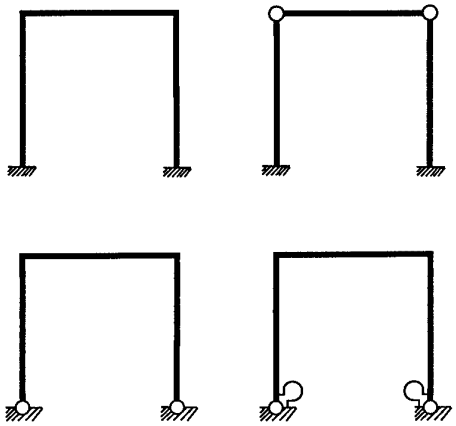


Figure 2.3: Example: Idealization of frame structure - specific mechanical models

Note: We have chosen, in a straight forward manner, beam elements. Why not shell elements; what is obout the structural connectors, the fasteners, the weldings, multidirectional (3d-) influences, etc. etc. ?

After a useful mechanical model has been selected, the next step is to find the proper loading cases and conduct a design procedure in accordance with the specific national standards. As well as the mechanical model contains idealizations there are also approximations and engineering assumptions within the loads, foundations, solid conditions, structural connections, assembling process, etc. etc. .

2.2.3.2 About engineering design

It is worth mentioning that there is a difference between engineering design tasks (e.g. the problem discussed above) and reliability tasks where the goal of investigation is a research project that is targeted on exactness.

Modeling is also part of the design process. Engineering design is related to statistical considerations concerning the safety of structures. Design engineers have to make sure that the ultimate limit of load capacity (and also the impairment of serviceability and durability) of the structure is not achieved. This is ensured by specific safety factors in the (national) standards.

Simplifications, e.g. in the mechanical model, may be accepted during the engineering design process, if we are on the *safe side* and the structure is still economical (or: Safety is payed!).

But also here, the question is: How do model-decisions, restrictions and simplifications influence the level of safety according to the postulated safety of the standards? The competition of engineering companies often drive us to approach the postulated safety of standards as best as possible. Large safety reserves are too expensive.

And therefore, it is important to ask how to get safe and reliable numerical simulations based on mechanical models that are close to reality at as best as possible.

Some examples of wrong design

Errors in engineering design can occur. Design by using finite element analysis is also prone to error. In ["Application of Computer Technology" by P. GARDENER, Forensic Engineering Conference, 1999.] a survey carried out by the American Society of Civil Engineers (ASCE) is mentioned. The survey covered 52 cases of error where the design process involved use of computers. It was found that 17% of the cases were affected by hardware error, 25% by software error and the remaining 58% by some form of user mistake:

1. hardware errors (17%),
2. software errors (25%),
3. user mistakes (58%).

"Some form of user mistakes" can be itemized as follows:

- wrong mechanical models implemented by the user,

- the "wrong method on the wrong place",
- "simple input errors": input mistakes, oversights, etc.,
- last but not least: misinterpretations of the numerical output.

These user mistakes are on the one hand mainly based on the lack of fundamental knowledge, and on the other hand based on time pressure and rush.

2.2.3.3 Numerical modeling - introductory example for hyperdynamic tasks

Special focus is done on hyper dynamics. An example, therefore, is a contact detonation problem that will be described in detail; see section 3.5.1.

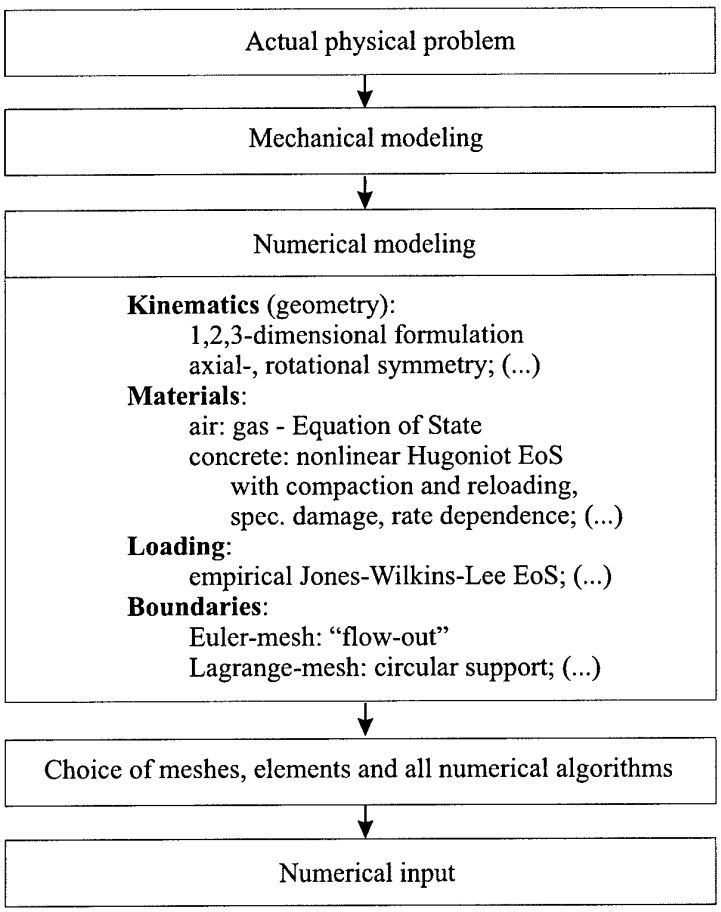


Figure 2.4: Modeling of a contact detonation problem, [32]

The procedure of modeling is shown in figure 2.4 (taken and modified from [32]).

In chapter 4 a more detailed guideline will be presented that accompanies the user for - amongst other things - the sake of proper modeling.

2.2.3.4 An input check list (in general)

The following list presents a general FE analysis input check list, taken (and modified) from [BENCHmark journal of NAFEMS, 07/2000]. It was not the goal here, to go into detail at every stage of the design process.

Table 2.1: input check list for a general FE ananysis

analysis type		elements missing	
units		elements duplicated	
extent of model		consistent normals	
material data		constraint equations	
co-ordinate system		symmetry constraints	
major dimensions		supports	
element types		boundary conditions	
real constants		load cases	
mesh density		summed mass	
element plots		master freedoms	
element shapes		front/band width	
internal edges		output options	

The check list in tab. 4.3 is general and not precise enough for specialized problems. But it is a guidance and it has to be modified and supplemented with respect to the problem that has to be solved (chapter 4).

2.2.4 Conclusion

Section 2.2 has - among other things - indicated the sources of errors that might be caused during the modeling process. In the following special focus is given to *sources of errors within the method* (section 2.3) and to *simplifications concerning material modeling* (section 2.4).

2.3 Sources of errors within the method

2.3.1 Finite methods - Introductory

Finite methods are approximation methods, because a variational principle adopting trial functions is used yielding a set of equations, here the equilibrium formulation in FEM:

$$\underline{K}(v) \cdot \underline{v} - \underline{F} \stackrel{!}{=} \underline{''0''} \tag{2.1}$$

The stiffness matrix $\underline{K}(v)$ is assembled representing both, material and system properties; $\underline{v}$ represents the unknown vector of nodal displacements; the load vector $\underline{F}$ has to be given by a specific load condition.

The nil ($\underline{''0''}$) in eq. 2.1 represents a mathematical truncation. It is dependent on the defined criteria of how $\underline{''0''}$ becomes almost 0.

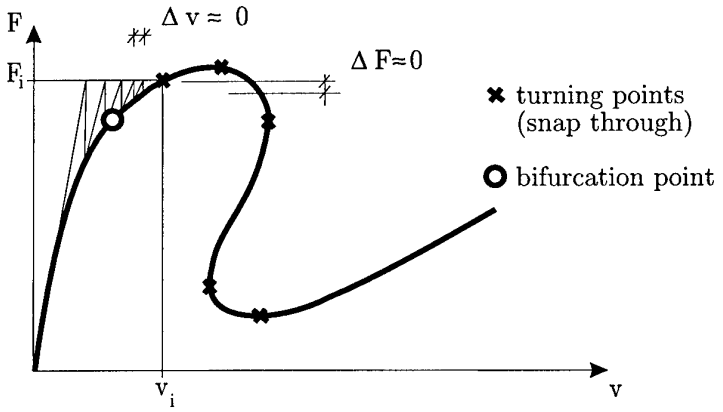


Figure 2.5: Load-displacement-path, internal truncation algorithm of FEM

Fig. 2.5 shows the trace of an incremental iterative algorithm driven by adaptive increments calculated from defined "norms". This "internal truncation algorithm" is based on the principle of exactness (section 3.4.3).

In the following, specific groups are listed that - at each case - represent **error levels**:

- structural component (rods, plates, ...),
- geometry of the numerical idealization,
- material formulation,

- contact algorithms,
- description of frictional effects,
- treatment of distorted elements,
- specific items, e.g. of hyper dynamics:
  - shock oscillations,
  - Lagrange/Lagrange interaction,
  - Euler/Lagrange coupling,
  - treating the multimaterial processor,
  - time step regulation in the explicit integration scheme,

→ On each level, possible errors have to be detected, treated and quantified separately!

2.3.2 A general example for approximation methods

As a first general example for approximation methods, the calculation of the circumference of a circle will shown {taken (and modified) from J.N. REDDY et al., [30]}:

The problem to estimate the perimeter of a circle of radius r might be solved by approximating it by line segments, whose lengths have to be summarized. This is a trivial example, but it illustrates some crucial ideas and steps involved in a finite element analysis.

The first step is the "discretization": The domain is the circumference of a circle that is represented as a collection of a finite number n of subdomains. These n line segments are called "elements" and the collection of them is called "finite element mesh". The elements are connected to each other at their points; so to call "nodes". A special case of this discretization is the uniform one, when all segments are of the same length.

The second step is to formulate the "element equations". Therefore a typical element, i.e. line segment, is isolated and its required properties, i.e. length, are computed by some appropriate means. Let h_e be the length of element Ω^e in the mesh:

$$h_e = 2r \cdot sin\frac{1}{2}\phi_e \ , \tag{2.2}$$

where r is the radius of the circle and $\phi_e < \pi$ is the angle subtended by the line segment.

In the third step an assembly of element equations and solutions have to be done. The approximate value of the circumference (or perimeter) of the circle is obtained by putting together the element properties in a meaningful way; this process is called the "assembly" of the element equations. In our example, it is computed by the sum of the lengths of all elements:

$$U_n = \sum_{e=1}^{n} h_e \ . \tag{2.3}$$

Then U_n represents an approximation to the actual perimeter u by using n segments.

If the mesh is uniform, $\phi_e = \frac{2\pi}{n}$ and h_e is always the same for each of the segments in the mesh. Then U_n becomes:

$$U_n = n \cdot \left(2r \cdot sin\frac{\pi}{n}\right) \ . \tag{2.4}$$

For this simple problem, we know the exact solution:

$$u = 2\pi r \ . \tag{2.5}$$

Thus, the "error" E_n in the approximation can be estimated by the following term:

$$E_n = \mid U_n - u \mid = n \cdot r \left(\frac{2\pi}{n} - 2sin\frac{\pi}{n}\right) = 2\pi r - U_n \ . \tag{2.6}$$

Here, E_n goes to zero as n $\rightarrow \infty$ that can be shown as follows. Letting $x = \frac{1}{n}$, we have

$$U_n = 2r \cdot n \cdot sin\frac{\pi}{n} = 2r\frac{sin\pi x}{x} \quad \text{and}$$

$$\lim_{x\to\infty} U_n = \lim_{x\to 0}\left(2r\frac{sin\pi x}{x}\right) = \lim_{x\to 0}\left(2\pi r\frac{cos\pi x}{1}\right) = 2\pi r = u \ .$$

[30]

Annotation:

This calculation is well understood as an "asymptotic convergence study". For this specific example, the circumference of a circle can be approximated as closely as we wish by a finite number of piecewise-linear functions. As the number of elements (segments), is increased, the approximation improves and the error in the approximation decreases (fig. 2.6, E$\rightarrow$0).

Certainly this circumference approximation is very simple, but this presentation has revealed some specific problems and steps that are also important when talking about finite methods. The additional problems are described in detail in the following chapters depending on the method used.

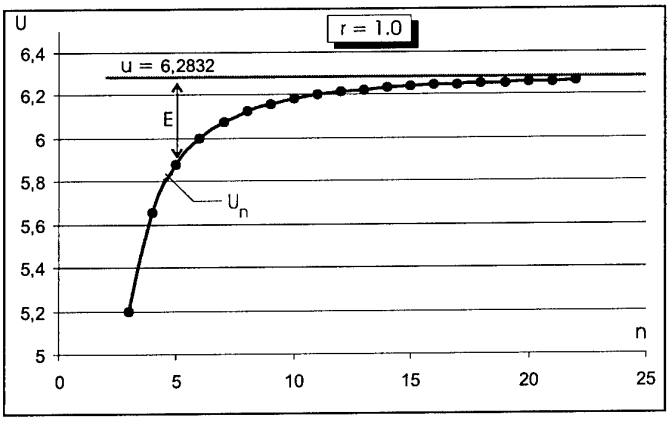


Figure 2.6: Asymptotic convergence of a simple circumference approximation

1. It is up to the user to define the Error E which can be accepted. From that depends the "size" of the problem.

2. If an element is too stiff, too weak, or shows locking, the solution might asymptotically converge to a wrong solution!

What is the proper method?

Uncounted papers and textbooks have been published dealing with theory and application of FE or FD methods. There are several computer codes which are commercially available to run on wide range of computer hardware. Meanwhile, FE analysis is playing a crucial role in research, development and practice. Computer simulation has become an important phase of design processes.

The key question is: "What is the proper method?". That leads to a comparison of different methods in order to gain information about both, advantages and disadvantages.

2.3.3 The finite element method (FEM)

2.3.3.1 Visible description

To apply the finite element method, a region in space is subdivided into a set of smaller subdomains or "finite elements". An approximate solution is then developed over each of these. This subdivision of a whole into parts allows accurate representation of complex geometries and nonlinear material behavior, for instance [30].

2.3.3.2 Choice of elements

Numerous types of finite elements are available within general purpose finite element codes. The choice of elements for a particular application will depend not only upon the more obvious matching of its shape attributes to those of the physical structure to be modelled, but also the less obvious matching of its displacement degrees of freedom (DOF) to be compatible with the structure's probable displacement behavior.

For example:
Although three-dimensional (3D) elements can be assembled to model any structure, care should still be taken to ensure that several layers of elements are present in regions subject to bending moments in order that meaningful stress values are obtained (GEBBEKEN & WANZEK [18], [35]). A mixture of elements within a model, each suited to a particular geometric shape, is preferable to attempting to use the same element types throughout. Thus, for example, slim two-dimensional (2D) rectangular elements with four nodes should not be used where slender beams in bending would be preferable. This is because the four noded element possesses only a linear displacement interpolation between its nodes. The element strain, which is the differential of the displacement, is therefore constant throughout the element. Thus, if in reality an appreciable strain gradient exists along the length of the element, serious incompatibilities will exist. The choice of a higher order, quadratic or cubic interpolation element (with extra face nodes) will considerably reduce this problem since, for instance, the quadratic element (with mid side nodes) will allow linear variation of strain and stress along and across an element to exist.

2.3.3.3 Element restrictions

After the choice of suitable elements has been made and a solution has been obtained, the analyst should be aware of possible deficiencies in the output information. Table 2.2 lists a range of elements which are commonly employed in FE analysis. The table lists the degrees of freedom or directions in which translational, U, and rotational, R, displacements or forces are available for an element together with a list of the direct, s, and shear, t, stresses produced by the element. The remarks column comments upon the limitations, for example, the stresses which are not given by the element. It may be seen, for instance, that shell elements do not record the presence of direct stresses or shear stresses through their thickness. This will be accurate enough for thin shells or for a thick shell with a large radius of curvature. However it may prove to be too restrictive in the case of a thick shell with a tight radius of curvature. In this case solid element modeling might well be considered.

Table 2.2: Range of elements commonly employed in FEM (PRINJA [?])

Standard Element Type	Active DOF	Output Stresses	Remarks
3D Solid (8-noded or 20-noded bricks.)	Ux,Uy,Uz	sx, sy, sz, txy, txz, tyz	Bending may require more than one 8-noded element through thickness or use higher order 20-noded bricks.
Axi-sym solid (3-noded or 4-noded)	Ur,Uz	sr, sz, shoop, trz	Bending may require more than one 3 or 4 noded el. through thickness or use higher order 6-noded or 8-noded elements.
3D Shell	Ux,Uy,Uz,Rx, Ry,Rz	sx, sy and txy in plane	Check validity for thin/ /thick shell assumption. No direct or shear stress through thickness.
Axi-sym. Shell	Ur,Uz, Rrz	smeridional and shoop	No direct or shear through thickness.
2D-Plane strain	Ux,Uy	sx, sy and txy in plane and sz	Through thickness strain is zero.
2D-Plane stress	Ux,Uy	sx, sy and txy in plane	Through thickness stress is zero.
Plate	Uz,Rx,Ry	sx, sy and txy in plane and t transverse	Membrane stress is zero.
3D-Beam	Ux,Uy,Uz,Rx, Ry,Rz	saxial , t torsion	No transverse shear stress
Truss	Ux,Uy,Uz	saxial	Only axial stress

2.3.3.4 Stress computation

As the finite element method is an approximation method, it is important to know that stresses are dependent on the location where they are calculated (REDDY [29]). It often happens (for isoparametric elements) that stresses are most accurate at GAUSS points of a quadrature point one order less than that required for full integration of the element matrix; especially for shear stresses.

For example, in a plane stress analysis the horizontal and vertical displacements are continuous, and in the analysis of a plate bending problem using the transverse displacement as only unknown variable, this displacement and its derivatives are continuous, too. However, this continuity does not mean that the element stresses are continuous across element boundaries (BATHE [2]). Of course, this problem diminishes when using a finer mesh.

2.3.3.5 (Further aspects)

Further aspects related to FE and error are:

- Locking effects,
- integration points,
- calculation of stress out of strain, (etc.)

(... they will not be discussed here ...)

2.3.3.6 Errors in FE solutions

(taken from REDDY [30])

The errors introduced into the finite element solution of a given differential equation can be attributed to three basic sources:

1. *Domain approximation error*, which is due to the approximation of the domain. In two- or three-dimensional problems involving non-rectangular domains, domain approximation errors are inevitably introduced into the FE solution. In general, these can be interpreted as errors in the specification of the data of the problem bacause we are solving the given differential equation on a modified domain. As we refine the mesh, the domain is more accurately represented, and, therefore, the boundary approximation errors are expected to approach zero.

2. *Quadrature and finite arithmetic errors*, which are due to the numerical evaluation of integrals and the numerical computation on a computer. When finite element computations are performed on a computer round-off errors of numbers and errors due to the numerical evaluation of integrals are introduced into the solution. In most linear problems with a reasonably small number of total degrees of freedom in the system, these errors are expected to be small.

3. *Approximation error*, which is due to the approximation of the solution. This error is inherent to any approximation method. It can be shown that the approximation error is zero for the single second-order and forth-order equations with element-wise-constant coefficients ([2], [30]).

2.3.4 The finite difference method (FDM)

{taken (and modified) from W.G. GRAY [23]}

2.3.4.1 Introduction

In elementary calculus the derivative is usually defined as the difference between values of a function at two points divided by the distance between the points taken in the limit as the distance approaches "0":

$$\frac{df}{dx} = lim_{\Delta x \to 0} \frac{f(x + \Delta x) - f(x)}{\Delta x} \ . \tag{2.7}$$

FD procedures involve the inverse of the above process such that a derivative based on a differential distance dx is approximated(!) as a difference based on some finite distance Δx. Of course in making the approximation a certain error(!) is introduced (section 2.3.4.2).

FDM is based on replacing the differential equation which holds for the entire domain under study with a number of discrete approximations to the differential equation which model the equation at selected points. The mentioned selection of points within this discrete approximation is commonly understood as **discretization**. Thus special focus will be taken on this matter; see later.

Another basic of this method is the dependency of each node on it's neighbours. Here a certain degree of dependency on the nearby points has to be taken into account. A simple approximation often used is that one point may only depend on the immediate neighbouring points. A complex approximation conceivably could depend on all other points. Thus although FDM utilizes local approximations, it is possible for points throughout the entire domain to contribute to the local approximation.

A simple example, one-dimensional:

An approximaton on an 1d-interval $[x_{i-2} \leq x \leq x_{i+1}]$, for example, is formulated as follows:

$$\hat{\mathrm{f}} = \sum_{j=-2}^{1} f_{i+j} \prod_{k=-2;\ k \neq j}^{1} \frac{(x - x_{i+k})}{(x - i + k)} \ ; \tag{2.8}$$

where $\hat{\mathrm{f}}$ is the approximation to a function f. In this special example, all nodes between x_{i-2} and x_{i+1} (four nodes) have been taken into account. Thus, three derivatives of $\hat{\mathrm{f}}$ can be formulated:

$$\frac{d\hat{\mathrm{f}}}{dx} = \sum_{j=-2}^{1} f_{i+j} \sum_{m=-2;\ m \neq j}^{1} \frac{1}{(x_{i+j} - x_{i+m})} \prod_{k=-2;\ k \neq j,m}^{1} \frac{(x - x_{i+k})}{(x_{i+j} - x_{i+k})} \ ; \tag{2.9}$$

$$\frac{d^2\hat{f}}{dx^2} = \sum_{j=-2}^{1} f_{i+j} \sum_{m=-2;\ m\neq j}^{1} \frac{1}{(x_{i+j} - x_{i+m})} \sum_{n=-2;\ n\neq j,m}^{1} \frac{1}{(x_{i+j} - x_{i+n})} \prod_{k=-2;\ k\neq j,m,n}^{1} \frac{(x - x_{i+k})}{(x_{i+j} - x_{i+k})}; \tag{2.10}$$

$$\frac{d^3\hat{f}}{dx^3} = \sum_{j=-2}^{1} f_{i+j} \sum_{m=-2;\ m\neq j}^{1} \frac{1}{(x_{i+j} - x_{i+m})} \sum_{n=-2;\ n\neq j,m}^{1} \frac{1}{(x_{i+j} - x_{i+n})} \sum_{k=-2;\ n\neq j,m,n}^{1} \frac{1}{(x_{i+j} - x_{i+k})}; \tag{2.11}$$

Obviously, the approximations to the first and second derivatives depend on space. This means that different approximations will be obtained by different locations. The third derivative depends not on space and we obtain a constant value when using a four node approximation as presented here.

Therefore, the accuracy of the approximation increases by taking more nodes into account. And it decreases when we go to higher derivatives with an approximation using a finite number of nodes. Thus, we need a greater number of nodes for higher derivatives.

When considering equidistant ($x_{i+1} - x_i = \Delta x$) nodes and evaluating the derivatives at, x_{i-2} for example, we obtain:

$$\frac{d\hat{f}}{dx}(x_{i-2}) = \frac{-11f(x_{i-2}) + 18f(x_{i-1}) - 9f(x_i) + 2f(x_{i+1})}{6\Delta x} \tag{2.12}$$

$$\frac{d^2\hat{f}}{dx^2}(x_{i-2}) = \frac{2f(x_{i-2}) - 5f(x_{i-1}) + 4f(x_i) - f(x_{i+1})}{\Delta x^2} \tag{2.13}$$

$$\frac{d^3\hat{f}}{dx^3}(x_{i-2}) = \frac{-f(x_{i-2}) + 3f(x_{i-1}) - 3f(x_i) + f(x_{i+1})}{\Delta x^3} \tag{2.14}$$

[23]

Numerical examples

We have selected four arbitrary functions as numerical examples; fig. 2.7 plots their curves. Their derivatives have been evaluated for the exact solution and for an FD-approximation.

Tab. 2.3 sumarizes the results comparing the exact solution and the FD approximation. For all functions two discretizations have been conducted, for four nodes each:

1.) $\Delta x = 1.0$; from $x_{i-2} = 2$ to $x_{i+1} = 5$, and

2.) $\Delta x = 2.0$; from $x_{i-2} = 1$ to $x_{i+1} = 7$.

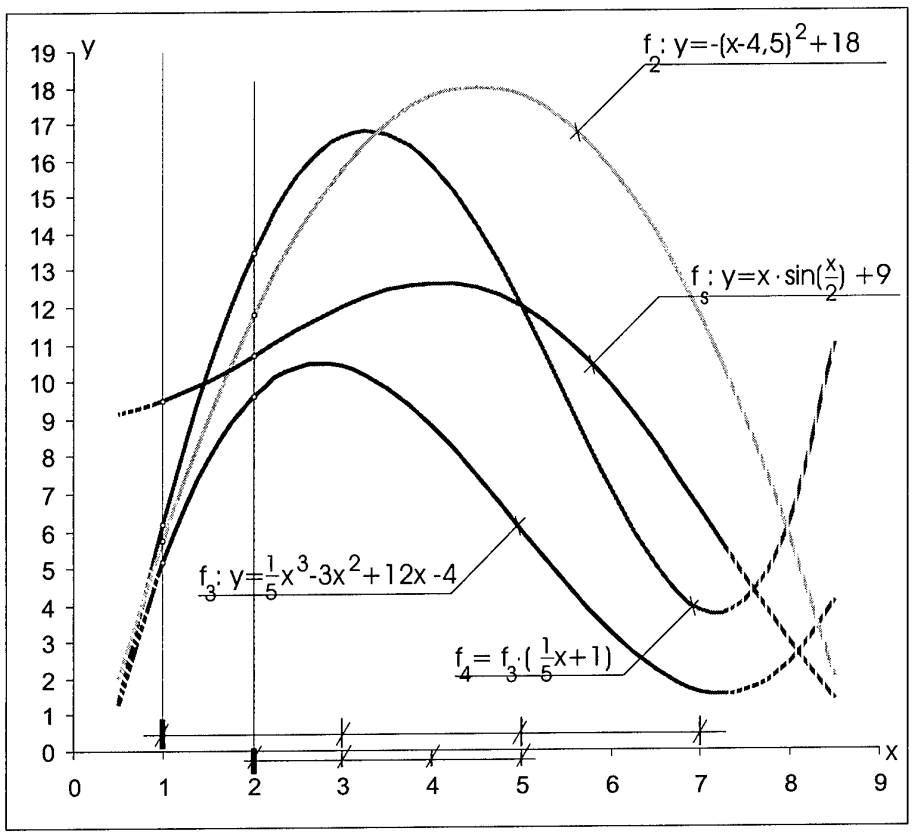


Figure 2.7: Selected functions: f_2, f_3, f_4, f_s

All these results have been evaluated at the first node x_{i-2} that is 2 for $\Delta x = 1.0$ and that is 1 for $\Delta x = 2.0$.

For the functions f_2 and f_3, there is no difference between the exact and the FD solution. f_4 and f_s have some significant differences instead.

Conclusion

The *accuracy* (see section 1.3.2) of FD approximations depends on

- the regularity of mesh,
- the function approximated,
- the locations where the derivatives are evaluated,
- the distance Δx that represents the mesh size,

Table 2.3: Selected functions and their derivatives: Exact solution and FD approximation

function and derivatives ...	exact solution (f', f", f"'); $x = x_{i-2}$	FD approximation ($\hat{f}$', $\hat{f}$", $\hat{f}$"'); $x = x_{i-2}$	error in %
$f_2: \ y = -(x-4.5)^2 + 18$	x=2	$\Delta x = 1.0$	x=2
... $\frac{df}{dx}(x_{i-2}) =$	5.0	5.0	0
... $\frac{d^2f}{dx^2}(x_{i-2}) =$	-2.0	-2.0	0
... $\frac{d^3f}{dx^3}(x_{i-2}) =$	0	0	0
$f_3: \ y = \frac{1}{5}x^3 - 3x^2 + 12x - 4$	x=2 / x=1	x=2 / x=1	x=2 / x=1
... $\frac{df}{dx}(x_{i-2}) =$	2.4 / 6.6	2.4 / 6.6	0 / 0
... $\frac{d^2f}{dx^2}(x_{i-2}) =$	-3.6 / -4.8	-3.6 / -4.8	0 / 0
... $\frac{d^3f}{dx^3}(x_{i-2}) =$	1.2 / 1.2	1.2 / 1.2	0 / 0
$f_4: \ f_4 = f_3 \cdot (\frac{1}{5}x + 1)$	x=2 / x=1	x=2 / x=1	x=2 / x=1
... $\frac{df}{dx}(x_{i-2}) =$	4.88 / 8.56	4.92 / 5.96	<1% / 30%
... $\frac{d^2f}{dx^2}(x_{i-2}) =$	-3.12 /-4.08	-2.64 /-4.96	15% / 21%
... $\frac{d^3f}{dx^3}(x_{i-2}) =$	-0.48 / -1.44	0.96 / 0.24	(±!)
$f_s: \ y = x \cdot sin(\frac{x}{2}) + 9$	x=2 / x=1	x=2 / x=1	x=2 / x=1
... $\frac{df}{dx}(x_{i-2}) =$	1.382 / 0.918	1.432 / 1.395	4% / 52%
... $\frac{d^2f}{dx^2}(x_{i-2}) =$	0.758 / 0.120	1.05 / -0.038	38% / (±!)
... $\frac{d^3f}{dx^3}(x_{i-2}) =$	-0.469 / -0.766	-0.489 / -0.626	4% / 18%

- the number of nodes that have been taken into account,
- the locations of these points, and
- the order of derivative.

In contrast to the FE method where one is looking at a problem from the global point of view, the FD method relies on a specific number of local approximations.

2.3.4.2 Error estimate

(taken from GRAY [23])

No error estimate is obtained directly when using polynomial interpolation to generate the difference expressions. But it is possible to determine the error by applying the difference expression successively to polynomials of higher degree until an error is detected. Then the dependency of this error on the grid size and the derivatives of the polynomial may be obtained.

This method in general reveals the truncation error E of the method. This can be well formulated in the special example from above by simplification of equations 2.12-2.14:

$$E = \frac{(6\alpha^2 - 6\alpha + 1)}{12} h^2 \frac{d^4 f}{dx^4} \,. \tag{2.15}$$

Herein α represents a certain position between the interpolation points, $x_{i+\alpha}$, where α can be choosen such that $0 \leq \alpha \leq 1$ and $h = x_{i+1} - x_i$.

2.3.4.3 Quadrilateral elements

Of course there are lots of formulations to approximate the state variables with respect to elements. In FD, most commonly a quadrilateral element approach is used; especially when using wave propagation codes: Hydrocodes (section 3).

A central difference scheme ([23], [2], [30], ...) is usually adopted within the FD method. The elements are commonly defined as quadrilaterals. It is assumed that the state variables (p, s_{ij}, ρ, i) are constant within an element.

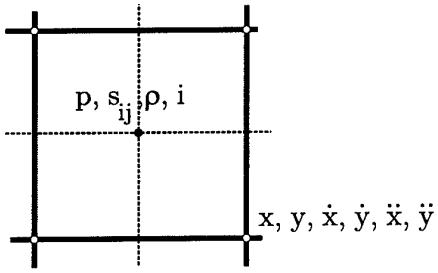


Figure 2.8: Quadrilateral element: Location of variables

Deformations, velocities and accelerations are evaluated at each corner node. Pressure, density, internal energy and the stress are parameters that are evaluated in the cell center (fig. 2.8). That means that the integration of the stress divergence over the element within the conservation of momentum (chapter 'Hydrocodes' 3, equ. 3.1), for example, is simplified by assuming that the stress is constant over the element. Therefore, very small element sizes are demanded when using the FD method.

2.3.4.4 Boundary and symmetry problems

Especially the FDM includes problems at boundaries and at the axis of revolution when using axial symmetry. This has been described in detail by BENSON in [3] with special respect to wave propagation simulations.

2.3.5 Comparison of FEM and FDM - an overview

Sections 2.3.3 and 2.3.4 have demonstrated that finite element and finite difference methods are numerical procedures which arise from different governing equations but which have more similarities in final application than casual inspection might reveal.

Before making a comparison of both methods, a numerical analyst must somehow ensure that he is using each method to best advantage. A comparison of a particular FE method with a particular FD method will not yield preference of FEM or FDM in general. Discussions which argue that one method is better than the other in fact often reflect that the author has merely utilized and programmed one method better than he has the other or he in fact prefers one method from his specific educational point of view.

But each method, FDM and FEM, has got it's special features which may be desirable for a particular application. Therefore, tab. 2.4 should provide a reasonable basis for categorizing a method as primarily FD or FE.

By this at hand, the user must decide, which method is best to apply for his specific task.

Table 2.4: Categorizing FEM and FDM (W.G. GRAY [23])

Finite Element Method (FEM)	**Finite Difference Method (FDM)**
Approximates the functions themselves.	Approximates derivatives of functions directly.
Provides global approximations which are restricted to neighborhoods of the grid to whatever degree desired.	Provides approximations at points which borrow information from neighboring points to whatever degree desired.
Structure of the method readily lends itself to irregular curved grids.	Traditionally uses a regular mesh; often only even a rectangular one.
Approximations developed from families of basis functions and integration over the grid.	Approximations developed via curve fitting for TAYLOR series expansions.
Resultant difference expression provided implicitily to the code which performs the integrations. Approximation is buried in the integrals.	Resultant difference expression explicitly provided by the programmer to the code. Approximation my be "seen".
Nodes included in discrete approximations determined by basis functions, integration rule and weighting fuctions.	Complete freedom to selected nodes to be used in a discrete approximation provided.
Even on a regular grid, different approx. may be made at different nodes (e.g. 9-node Lagrangin elements).	On a regular grid, similar approximations are made at different nodes.
Difference expressions are often written in terms of function values and derivatives of the functions.	Difference expressions are generally in terms of function values only.
...	...

Table 2.5: (continued)

Finite Element Method (FEM)	**Finite Difference Method (FDM)**
...	...
Though typically weighted over different coordinates, derivatives may sometimes be lumped by selection of an appropriate nodal integration formula (e.g. trapez.-rule for bilinear elements).	Though not typically done, derivatives with respect to one independent variable may be weighted over another variable (e.g. a time derivative approx. may be a sum of time derivatives evaluated at different spatial locations).
A staggered grid is virtually impossible because of grid irregularities.	A staggered grid is easily implemented because of regular rectangular nodal placement.
Moving boundary problems are conceptionally straightforwarde.	Moving boundary problems are traditionally difficult.
Functional implanting may minimize need for fine mesh near steep gradients.	Large gradients require a fine mesh for resolution. More elements are required.
Data input often is complex and undiscovered data errors can be a cause of trouble.	Data input may be simple because of regularity.

2.4 Simplifications concerning material modeling

Depending on the real material behavior, we have to select the proper material model. Material behavior can be described as:

- linear elastic,
- non-linear elastic,
- elasto-plastic,
- viscous,
- and others (and combinations).

Choosing the wrong model is obviously a source of error.

Fig. 2.9 shows some basic reological models related to their specific material behavior.

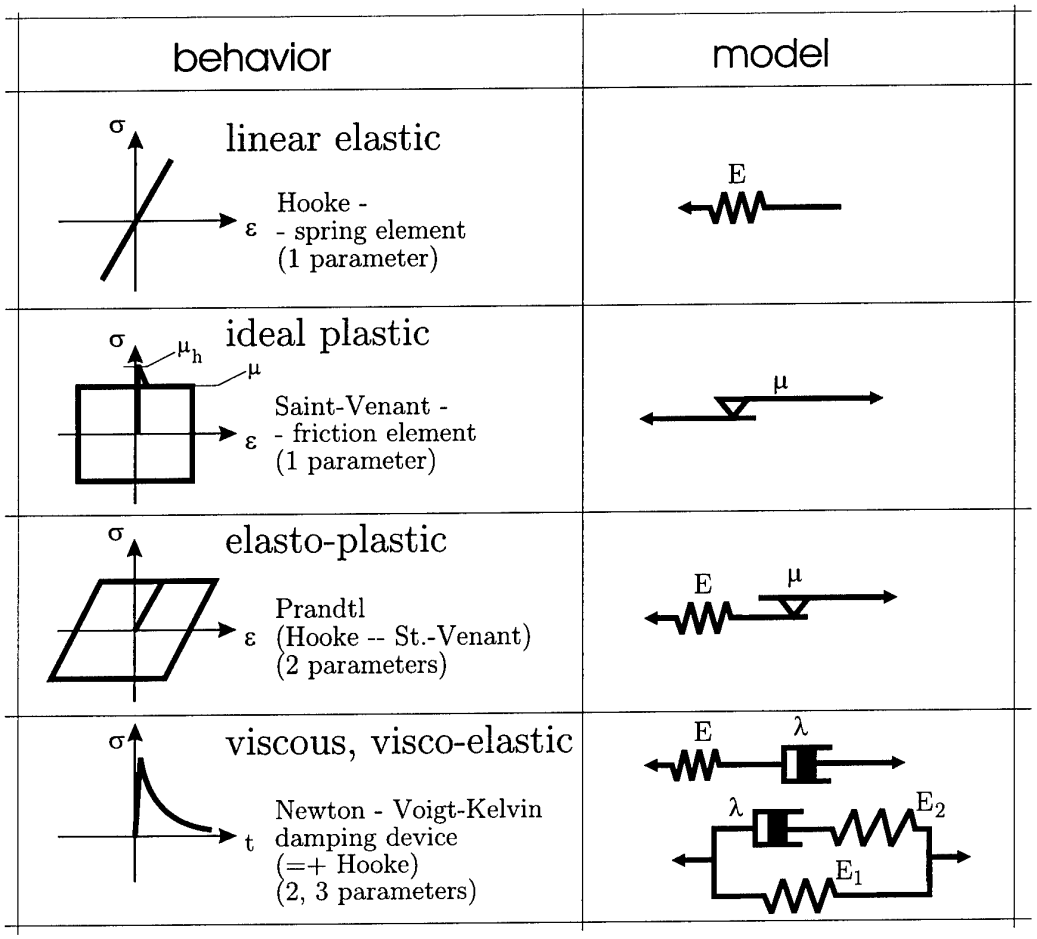


Figure 2.9: Behavior and models of basic material formulations

When integrating material models into finite methods, it is common practice to simplify in certain points. Although simplifications are usual and always done, one should be aware of the consequences. Nevertheless, there are unavoidable simplifications also in material modeling.

The following examples are not a complete review of all approaches that might be possible in the field of material modeling, but they are implemented in almost every commercial code and are broadly used.

We have to insinuate that most users have not realized the consequences resulting from this. To understand us correctly, it is not a goal here to disrepute these methods. But doing simplifications as presented now, one has got a more or less "rough estimate" of the problem to be solved, before any calculation has been started.

2.4.1 Example 1: HOOKE's law of elasticity

Up to a certain load level - the elastic limit -, the material response can be understood as ideally elastic. In this case HOOKE's law of elasticity is commonly used. This approach is necessarily based on the homogenization principle (chapter 1, fig. 1.4).

HOOKE's law can be written as:

$$\sigma_{ij} = E_{ijkl}\,\epsilon_{kl}\ , \tag{2.16}$$

wherein E_{ijkl} is the elasticity tensor.

This general formulation contains 81 independent material parameters for an elastic, anisotropic material.

By progressively conducted simplifications the number of 81 independent parameters in eq. 2.16 can be reduced to 2 which leads to an isotropic formulation:

$$\begin{Bmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \\ \tau_{12} \\ \tau_{13} \\ \tau_{23} \end{Bmatrix} = \begin{bmatrix} E_{11} & E_{12} & E_{12} & 0 & 0 & 0 \\ E_{12} & E_{11} & E_{12} & 0 & 0 & 0 \\ E_{12} & E_{12} & E_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{E_{11}-E_{12}}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{E_{11}-E_{12}}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{E_{11}-E_{12}}{2} \end{bmatrix} \begin{Bmatrix} \epsilon_1 \\ \epsilon_2 \\ \epsilon_3 \\ \gamma_{12} \\ \gamma_{13} \\ \gamma_{23} \end{Bmatrix} \tag{2.17}$$

The (only) two paramaters of this elastic law for isotropic material are called Lamé-constants λ and μ. They depend on values necessarily to be derived from experiments, the modulus of elasticity E and the shear modulus G; or the modulus of compression K and the POISSON's ratio ν.

$$E_{11} = \frac{E(1-\nu)}{(1+\nu)(1-2\nu)}\ , \tag{2.18}$$

$$E_{12} = \frac{E\nu}{(1+\nu)(1-2\nu)}\ . \tag{2.19}$$

$$\lambda = \frac{E\nu}{(1+\nu)\,(1-2\nu)} = E_{12}. \tag{2.20}$$

$$\mu = G = \frac{E}{2(1+\nu)} = \frac{E_{11}-E_{12}}{2}. \tag{2.21}$$

The procedure of simplification to get this law is shown in [17], for example. tab. 2.6 gives an overview of the steps that lead to different material laws; from the general elasticity law to the

two-parameter model that is used by most numerical codes for isotropic elasticity.

Table 2.6: Material definitions and number of independent material parameters [17]

material	number of independent material parameters
arbitrary: no simplification	81 (36)
anisotropic	21
monocline	13
orthotropic	9
transversal isotropic	5
isotropic	2

Annotation: Most numerical codes, especially hydrocodes, offer only the simple elasticity law with two parameters. As we know, concrete is a highly anisotropic material and, therefore, the material model for concrete should have at least 21 independent material parameters (tab. 2.6). If we simplify the concrete material by homogenization techniques, we should be aware of the possible error.

2.4.2 Example 2: POISSON's ratio

Reflecting the POISSON's ratio leed to a change in theory; [32].

The POISSON-ratio ν can be calculated from experimental measurements taken from the uniaxial tension test.

$$\nu := \frac{\epsilon_y}{\epsilon_x} = \frac{-\frac{\Delta l_y}{l_y}}{\frac{\Delta l_x}{l_x}} = -\frac{\Delta l_y \, l_x}{l_y \, \Delta l_x} \tag{2.22}$$

$$\epsilon_y = -\nu \epsilon_x \tag{2.23}$$

$$\epsilon_z = -\nu \epsilon_x \tag{2.24}$$

wherein

ν : POISSON's ratio,

$\frac{1}{\nu}$: POISSON's constant.

For examle, the static values are:

$$\nu^{steel} \approx 0.3 \tag{2.25}$$

$$\nu^{concrete} \approx 0.2 \quad (0.12 - 0.46) \tag{2.26}$$

While steel is highly homogenious, concrete is absolutely not homogenious, and the ingredients change due to the ordered concrete quality. If someone models a highly homogenious material the quantity of the POISSON's ratio is almost a constant. Modeling concrete, and setting $\nu = 0.2$ means producing an input error up to 240%.

Transformation into a stress-explicit description yields:

$$\epsilon_{1,1} = \frac{\sigma_1}{E} \tag{2.27}$$

$$\epsilon_{1,2} = -\nu\epsilon_2 = -\nu\frac{\sigma_2}{E} \ , \tag{2.28}$$

$$\epsilon_{1,3} = -\nu\epsilon_3 = -\nu\frac{\sigma_3}{E} \ , \tag{2.29}$$

$$\epsilon_1 = \frac{1}{E}[\sigma_1 - \nu(\sigma_2 + \sigma_3)) \ , \tag{2.30}$$

$$\epsilon_2 = \frac{1}{E}[\sigma_2 - \nu(\sigma_1 + \sigma_3)) \ , \tag{2.31}$$

$$\epsilon_3 = \frac{1}{E}[\sigma_3 - \nu(\sigma_1 + \sigma_2)) \ , \tag{2.32}$$

Inversion yields:

$$\sigma_1 = \frac{E}{(1+\nu)(1-2\nu)}[(1-\nu)\epsilon_1 + \nu(\epsilon_2 + \epsilon_3)] \ , \tag{2.33}$$

$$\sigma_2 = \frac{E}{(1+\nu)(1-2\nu)}[(1-\nu)\epsilon_2 + \nu(\epsilon_1 + \epsilon_3)] \ , \tag{2.34}$$

$$\sigma_3 = \frac{E}{(1+\nu)(1-2\nu)}[(1-\nu)\epsilon_3 + \nu(\epsilon_1 + \epsilon_2)] \ , \tag{2.35}$$

Change in volume:

$$dV + \Delta dV = dx(1+\epsilon_1)\ dy(1+\epsilon_2)\ dz(1+\epsilon_3) \ . \tag{2.36}$$

Hence, the volume strain:

$$\begin{aligned} e \ &:= \ \frac{\Delta dV}{dV} = \frac{dV + \Delta dV \ - dV}{dV} \\ &= \ \frac{dx(1+\epsilon_1)\ dy(1+\epsilon_2)\ dz(1+\epsilon_3)}{dx\ dy\ dz} \\ &= \ \underbrace{\epsilon_1 + \epsilon_2 + \epsilon_3}_{e_{linear}} + \underbrace{\epsilon_1\epsilon_2 + \epsilon_2\epsilon_3 + \epsilon_3\epsilon_1 + \epsilon_1\epsilon_2\epsilon_3}_{e_{nonlinear}} \end{aligned} \tag{2.37}$$

The volume dilatation:

$$\Rightarrow \ e_{linear} = \frac{1-2\nu}{E}(\sigma_1 + \sigma_2 + \sigma_3) = \frac{1-2\nu}{E}\ 3\sigma_m + 3\alpha_T\vartheta \ , \tag{2.38}$$

where

$$\sigma_m = \frac{1}{3}(\sigma_1 + \sigma_2 + \sigma_3) \tag{2.39}$$

$$= \text{mid. (average) stress} = \text{compression stress:}$$

$$\Rightarrow \; e(= e_{linear}) = \frac{\sigma_m}{K} \; , \tag{2.40}$$

wherein K is the modulus of compression.

For K follows that POISSON's ratio only can reach values between $0 \leq \nu < 0.5$. Figure 2.10 shows the functional of the modulus of compression K over ν. $\nu \rightarrow 0.5$ yields $K \rightarrow$ infinity.

$$\begin{aligned} \sigma_m &= constant \\ e &= 0 \\ \Rightarrow K &\rightarrow \infty \\ \nu &\rightarrow 0.5 \end{aligned}$$

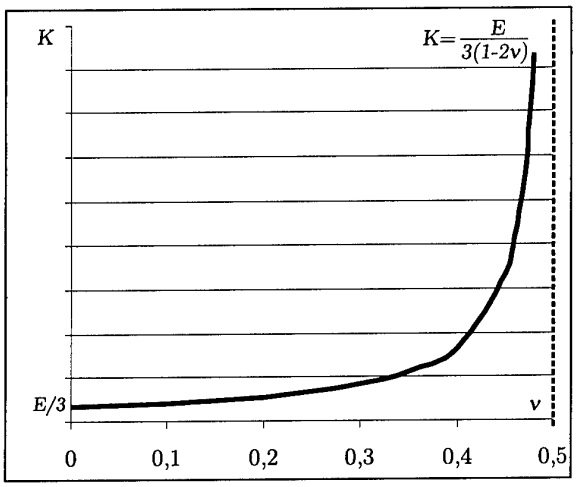


Figure 2.10: Modulus of compression K vs. ν

Conclusion:

For $\nu \rightarrow 0.5$ theory must change. For ν is close to 0.5 means, physically, approaching incompressible materials. This requires a constitutive law for the pressure, the hydrostatic part. So we must extent the classical theory of continua.

Consequence: Split of the stress tensor

Because of this, many methods are based on the additive split of the stress tensor into a hydrostatic part and into a deviatoric part. The first describes the change in volume and - as we know from experimental studies (on metals) - has no influence on plastic yielding. The latter describes the shape deformation part. Applying this for concrete needs an extention: While steel or rubber is almost incompressible, concrete is compressible due to the collapse of concrete's material matrix by applying high pressures (p>20 kbar). Thus, the hydrostatic part has to be considered, accompanied by an Equation of State (EoS).

Chapter 3

Wave propagation codes - Hydrocodes

3.1 Introduction

3.1.1 Available Hydrocodes

Nowadays, numerous commercial hydrocodes are available for almost everyone (tab. 3.1). AUTODYN is one of them, and used by the authors.

As explained before, one should always be aware of the method that is used by the software. Otherwise, a meaningful use is impossible. The user is always confronted with the key question "which software is the best for my problem".

Software was mostly developed for special purposes, and, therefore, there is no general purpose software available. Because of the competition between software developers & vendors they often promise too much (section 1.3.4).

But, it is the user's duty to ensure that his numerical result and that the interpretation of the result (section 3.2) is correct. Not knowing the "secrets" of the source code worsens this problem.

Table 3.1: Available hydrocodes, taken from MEYERS1994 [26], modified and supplemented

hydrocode	properties	developer
TOUDY	Lagrange-processor	Sandia Nat. Labs.
HEMP	Lagrange-processor	Lawrence Livermore Nat. Labs.
STEALTH-2d,3d	Lagrange-processor	Science Appl. Inc.
PRONTO-2d,3d	Lagrange-processor	?
MESA-2d,3d	Euler-processor	Los Alamos Nat. Labs.
PAGOSSA-3d	Euler-processor	Los Alamos Nat. Labs.
JOY-3d	Euler-processor	Lawrence Livermore Nat. Labs.
DYNA-2d,3d	Lagrange-processor	Lawrence Livermore Nat. Labs.
LSDYNA2d,3d	Lagrange-, Euler-processor	Lawrence Livermore Nat. Labs.
CALE-2d	Lagrange-processor	Lawrence Livermore Nat. Labs.
CAVEAT	?	Los Alamos Nat. Labs.
CTH-2d,3d	Lagrange-processor	Sandia Nat. Labs.
PICES-2d,3d	Lagrange und Euler gekoppelt	Physics Inernational
CRALE-2d	Arbitrary Lag./Euler-processor	?
CSQ II-2d	Euler-processor	Sandia Nat. Labs.
EPIC-2d,3d	Lagrange-processor	Honeywell
NIKE-2d,3d		Lawrence Livermore Nat. Labs
ZEUS	Lagrange-processor	Segletis & Zukas
AUTODYN2D	Lagrange und Euler gekoppelt	Century Dynamics
AUTODYN3D	Lagrange-, Euler-processor	Century Dynamics
TDL MADER	Lagrange-processor	C. Mader
DYSMASS	Lagrange-, Euler-processor	IHBG
SHARK	Euler-processor	
...	...	...

3.1.2 Why and when hydrocodes are used

There is obviously an increasing demand by building owners to design their structures for hazard loadings. These loadings are caused by explosion, impact, penetration and perforation, for example, and produce high pressures in the kilobar region within microseconds in the material.

Structural dynamics methods are well known but insufficient for hyper dynamics (section 1.4). Thus, wave propagation codes (hydrocodes) are nowadays applied.

It is not a trivial task to numerically predict damage and fracture caused by hyper dynamic impacts. The fields of interest where hydrocodes are applied are - for example -:

- fluidal flow simulations,
- gas dispersion,
- free explosions in air,
- contact explosions on structures,
- impact, penetration and perforation phenomena.

Some examples will be shown in the sections bellow (sections 3.5.1 and 3.5.2).

Actually, hydrocodes are the most powerful numerical tools for the numerical study of shock and impact phenomena. But up to now, it is impossible to totally replace all experimental investigations by (cheaper) hydrocode simulations. Experiments are still necessary, for benchmarking, for calibration of material parameters, etc. .

3.2 Pre- and post-processing, interpretation of results

In order to use finite methods effectively, software tools must be user-friendly. Therefore, user graphical interfaces, pre- and post-processors have been developed. But user-friendly does not mean that pre- and post-processors can replace the knowledge and experience of the user.

3.2.1 Pre-processing

Overview:

- Generation of geometrical models,
- generation of numerical models,
- possibly data transfer from CAD,
- implementing material data,
- specify units, methods, *etc.*,
- generation of meshes,
- check of elements and input,
- check of numerical models.

3.2.2 Post-processing

The treatment of numerically derived data, their sorting, combining and presentation/visualization in graphical form is referred to as *post-processing.* In the post-processing phase, results may be produced in the following forms; see "How to - Interpret Finite Element Results" by BAGULEY & HOSE, NAFEMS publications:

- displaced shape plots,
- contour plots of displacements,
- plots showing reaction forces and moments,
- listing of stresses or strains sorted by ascending or descending magnitude,
- contour plots of stresses or strains,
- vector plots showing the directions of principal stresses,
- plots of stresses or strains along paths,
- plots of deflection, stress or strain against time,
- path integrals such as J-integrals for fracture mechanics.

3.2.3 Interpretation of results

The interpretation of results is a focal point!

Results from post-processing help the analyst to understand how the model behaves. To achieve the objective of the analysis it is necessary to translate these results into the behavior of a real structure. This may require adjustments to the results to allow for the differences between the model and the real structure, and this process is referred to as *interpretation.*

Increasing computer technology in connection with sophisticated pre- and post-processors offers both, **new chances and new risks**.

Besides calculations of huge problems, the **chance** is to lay a powerful tool in the user's hand which enables "easy" pre-processing and an extensive analysis of the results.

Risks lie, for example, in mistakes of pre- (input problems) and post-processing (misinterpretations) made by the user and/or clients. There is also a significant risk to use a wrong model or the wrong method. Using tools as black boxes prevents insight into what one is actually doing which increases this problem.

The code developer should clearly state how the program treats the data; e.g. "shaping" or "smoothing" of data at integration points into contour plots etc. . Traceability and transparency (section 1.3.2) of tools are necessary for the evaluation of methodical inherent errors.

3.3 What is "code validation"?

3.3.1 Introduction

Scientists, code users and developers have of course recognized that *validation and verification* is crucial for the reliability and safety of numerical simulations. Within the last two decades the term *"code validation"* has been used increasingly (see "Preface" at page 1).

But code validation has, however, become neither a common term nor does it even have a standardized and commonly understood content. "Code validation" is approached in different ways and in different intensity; depending on the specific problem to be solved (here: hyperdynamic problems), the method used, the different goals of the interested parties (section 1.3.4), the education of users and developers, and the available budget.

For example, HILLS and TRUCANO describe in [24] a *statistical validation of engineering and scientific models.* Herein the focal point concerning **code validation** is the match between experiment and numeric after plotting their results. The key question that HILLS et al. approach is: "When is the agreement between experimental measurement and model prediction good enough?"

3.3.2 How to find a proper 'definition'

Validation is a confirmation, through the provision of objective evidence, that the requirements of a specified intended use or application have been fulfilled (section 1.3.2).

Here, the key *requirement* is to *fulfill* the essential accuracy of numerical results. Therefore, we propose the following:

1. Plausibility studies of various problems in order to know the limit of applicability (section 3.3.3).

2. Testing codes against numerous (critical) credible(!) experimental results: Benchmarking (section 3.3.4).

3. Testing codes against each other. Do not use only one commercial code!

4. Plausibility testing of the results by hand calculations, known formulars (if it is possible).

But *objective evidence*, that numerical results are safe and reliable, cannot be ensured only by the user nor only by the code developers each on their own. Beyond the proper interaction of all interested parties (section 1.3.4) it is also important, that code developers, code vendors, code users and their partners *validate* each other.

3.3.3 A specific plausibility study

The following might be done by the user as a first step of code validation:

For example, characteristic material data has been reliably obtained by a set of flyer plate impacts: $EoS: \; U_S = a + b \cdot u_p$ (e.g. [?]). Thus, a and b are the parameters in the shock velocity - particle velocity relation.

The result of a numerical simulation – using exactly the same conditions (materials, ...) as in the experiment – will also lead to a shock velocity - particle velocity relation: $EoS^*: \; U_S = a^* + b^* \cdot u_p$.

Such a study can be understood as a combination of the first two items of the 'definition' above (section 3.3.2).

"To all intents and purposes", the experimental data (a and b) and the numerical result (a^* and b^*) should not differ from each other. But an exact match between testing and numeric ($a = a^*$, $b = b^*$) is only an ideal case that we cannot expect. Indeed, a (b) and a^* (b^*) will differ most likely.

But why?

The answer to this question is the answer to "How can we conduct code validation?".

Code validation is not "only matching EoS with EoS^*" and "be satisfied when the difference is of about less than 5%" (for example done by *curve fitting*). Proper code validation is the answer to the question "where do the 5% come from?". Sections 3.4 and 3.5 try to give answers.

3.3.4 An overall data base board for benchmarking

The following proposal for an overal data base board is partly taken from the "DFL Data Base for RCS Computational Code-Validation" [13].
In our opinion it could be well transfered to our code validation problem. For example an overall database board for benchmarks.
Thus, it has been modified and supplemented here for the general purpose to be discussed.

A data base board is intended to streamline the process of establishing confidence in a given computational code. The data base contains experimental as well as numerical results. The data has to be for many targets, from very simple problems to more complex objects. Complexity might rise by both larger setups and more complicated problems like hyper dynamic impacts. Users and code developers should be able to download the numerical values of the data as needed establishing the accuracy of a new code and in testing its limitations. Code users wishing to establish confidence in a given code can obtain measured data for comparison with their own discretizations and computations.

We should create user groups of common interest beyond the limit of usergroups for a specific software package.

Further, users and developers have to be invited to contribute their computations and measurements to the data base. The intention is that a user wishing to examine the evidence supporting the accuracy of a certain code can look into the data base and find computations with that code compared with measurements for various targets, including the details of the discretization. This may save new users the expense of extensive code validation studies of their own, as such studies are readily available. Further, a new user can examine the details of the discretizations available on the data base to learn to build his own models effectively.

Another objective is to allow a user to compare the performance of various codes to choose the one most suitable for a given application. Thus, if a given target has been solved using a number of different codes, the user can examine the predicted by the various codes in relation to one another and to the measured results. If such comparisons are available for a variety of targets, the user has quick access to a comprehensive comparison of the performance of the various computational techniques available for that problem.

Those developing a code may wish to use this data base to demonstrate their code's performance relative to other codes. By contributing data to data base computed with their code for various problems, the capabilities of the code are exhibited, relative to other methods. Potential users shopping for a code can evaluate various codes one against the other. There is an advantage for both for users and for developers.

A contribution to the data base has to have four key parts:

- identification,
- problem,

- method and
- data.

The problem being addressed must be clearly identified, either as one already on the data base or as a new problem. The method used for solving the problem must be fully described. A certain instance has to proof every ingoing contribution before distributing it. Queries from the board chair are imperative there. There also should be a detailed questionnaire to be filled out by one who wants to send a contribution. In this kind of form also general information might be asked for; e.g. information about the computer resources including the disc space needed, the memory requirements, and the running time on a specific processor. When measured data is submitted to the data base a description of the measurement facilities, the instrumentation and the methods used have to be included. To get information about experimental results without an detailed description of the method used is for nothing! The problem geometry must be described in detail, including a drawing if required for clarity. Measured data is desirable if the problem is to be used as a reference for code validation, although computations alone should be posted as an invitation to others to solve the geometry with their code and compare with the results already posted for code validation purposes.

[13]

Specific references

First of all, the "DFL Data Base for RCS Computational Code-Validation" of the Canadian Space Agency has to be mentioned. The text above is partly taken from this organisation.
[http://lucas.dfl.crc.ca/rcs/rcs.html]

The "CFD CODE VALIDATION DATABASE" provides a focus for CFD code validation in areas deemed most important to U.S. aerospace industry.
[http://iadt.arc.nasa.gov/database/1describe.html]

"The development of standards for code validation and verification."
[http://www.aiaa.org/information/technical/rev-as.html]

Institute for Mathematics and its Applications (IMA), Sandia Nat. Lab.: "Code validation as a reliability problem" by T. G. Trucano.
[http://www.ima.umn.edu/reactive/abstract/trucano1.html]

Sandia Nat. Lab.: "Description of the Sandia Validation Metrics Project" by TRUCANO et al. [34]

3.4 The basics of hydrocodes

In this section, first of all, a brief overview of the theoretical background of hydrocodes will be given (subsection 3.4.2). Afterwards important demands are done that are essential for all codes used (subsection 3.4.3). Subsections 3.4.4–3.4.7 treat our experience with hydrocodes and, therefore, some specific proposals are made.

3.4.1 Waves, compression waves, shock waves

The theory of waves is important to understand also hyper dynamic phenomena. But this will not be discussed in detail here. For such basics we refer to [26], for instance.

3.4.2 Theoretical background

Basically, it is important to consider all aspects mentioned in chapter 2 when talking about finite methods.

The most hydrocodes are based on the FD method (section 2.3.4) for time discretization, especially when shock wave phenomena are the key subject. In addition they are in general "explicit codes" with respect to the solution in time (explicit integration).

There are, however, some additional aspects with hydrocodes. While FE codes are usually based on the direct solution of the equilibrium equations, hydrocodes are commonly based on the direct solution of the conservation equations for mass, momentum and energy. Thus, their governing equations are different. The conservation formulas have to be fulfilled simultaneously in every time step during the computation.

In order to well understand the development of shock, eq. 3.1 includes the equations for the hydrostatic case. The pressure is the predominant action here. Eq. 3.1 can also be applied to the one-dimensional stress state. Eq. 3.1 is valid for all situations where the deviatoric part can be neglected compared to the hydrostatic pressure part. This is common practice when solid material under high pressure is under consideration. Therefore, eq. 3.1 has been derived by directly using the instantaneous shock condition which is shown in fig. 3.1.

$$\begin{array}{lll} \text{Mass} & \rho\,(U_s - u_p) = \rho_0\, U_s & \text{(a)} \\ \text{Momentum} & p + \rho\,(U_s - u_p)^2 = p_0 + \rho_0\, U_s^2 & \text{(b)} \\ \text{Energy} & e + \frac{1}{2}\,(U_s - u_p)^2 = e_0 + \frac{1}{2}\, U_s^2 & \text{(c)} \end{array} \tag{3.1}$$

The initial parameters (p_0, ρ_0, e_0) are known. The atmospheric overpressure p_0 is very small

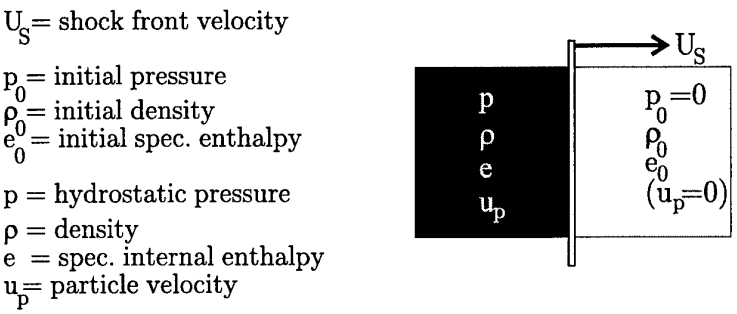


Figure 3.1: Shock front

in comparison with the maximum pressure and is usually neglected. The initial internal energy $i_0 = e_0 - \frac{p}{\rho}$ corresponds to the actual temperature. Finally, the four unknowns (p, ρ, $e(i)$, u_p) remain in three independent equations. That yields a lack of one equation. In general, any additional relationship between two unknown parameters can be taken into account. Usually a formula between pressure, density and energy is taken that is called Equation of State (EoS) (e.g. the authors in [19]–[22], [31], [32]).

There are some problems concerning the EoS. In this paper, it is impossible to go into detail here. Nevertheless, one should be aware that the EoS can only be determined by experimental investigations.

Eqs. 3.1 (a)-(c) reveal that there is need to provide an additional constitutive material law of the form $\sigma = \sigma(p, \epsilon, \dot{\epsilon})$. The material strength is usually modeled by a failure surface $f = f(I_1, J_2, \theta(J_3))$. It will be derived from the theory of continuum mechanics.

For further information an theoretical details of hydrocodes we refer to relevant literature (e.g. [1], [3]).

3.4.3 Important demands to the hydrocode used

The following demands are essential for all numerical kernels of codes, but especially for wave propagation codes:

- Asymptotic convergence,
- robustness,
- numerical stability,
- accuracy,

- consistence.

3.4.3.1 Asymptotic convergence

– Discretization errors in finite methods –

Again, finite methods are approximate methods (section 2.3.2). Thus, methodical inherent errors have to be detected and reduced to an acceptable minimum. This is absolutely indispensable in order to obey the physical laws. If one does not, the numerical procedure might smear effects and afterwards one is unable to analyse and evaluate the numerical results with respect to the causes. In the worst case, the obtained numerical results are nonsense and just numbers free to any interpretation. Quantifying the value of an "acceptable minimum" is dependent on the kind of problem.

Every finite method has methodical inherent errors of discretization, spatial (mesh sensitivity) and in time (timestep). In order to produce safe and reliable numerical results, it is important to determine the methodical inherent aspects. In section 3.5, a detailed convergence study will be discussed, based on the convergence theorem:

If a partial differential equation is discretized by means of finite elements or finite differences, the numerical solution must monotonically converge to the exact solution of the mechanical model if and only if the element size and the timestep tend to zero.

This convergence theorem is based on the assumption that the selected finite elements work ... (no locking effects, etc.).

The main goal is to find a numerical model which is as coarse as possible and as fine as necessary. This can be a time consuming effort. Because of time pressure, if a comparative study has been done, often just 2 elementations are compared. With two values, one can generate a linear formulation but not a monotonic convergence. But there is an exception: If the results of two really different elementations do not differ more than 3% the "rough" mesh must be seen as acceptable.

To find the reasons of method inherent problems concerning convergence, stability, and sensitivity the theoretical background of the tool used has to be studied.

Important to know and to accept is the fact that, methodical inherent, there might exist some regions where no convergence can be adopted. An example is given in section 3.5.

3.4.3.2 Robustness

Robustness or smooth behavior: *Small variations must cause small changes in results!* Therefore, sensitivity studies for all relevant numerical parameters have to be taken into account.

The controll of robustness is important especially for hyper dynamic problems where the variation of the state variables is immense in a short duration of time. An example is shown in section 3.5.2 where *internal numerical parameters* in penetration problems are discussed.

In contact detonation problems this becomes evident when using Euler-Lagrange-coupling. Not only mesh sizes or the mesh size ratio (discussed in section 3.5.1.4) influence the results. Also the alignment between the Euler and the Lagrange mesh is important to consider. Using whole-numbered ratios cause changes in pressure–time plots that are physically not explainable ([32]). Therefore, we recommend a pre-study on robustness for the special problem that has to be solved. This has been done by the authors in [32], for example, for contact detonation problems (section 3.5.1.4).

3.4.3.3 Numerical stability

Numerical stability (of explicit (hydo-)codes, numerical damping, and others). Normally this can be assumed to be satisfied in commercial codes. ANDERSON describes the handling of numerical stability in detail in [1].

3.4.3.4 Accuracy

Accuracy is here referred to the internal method's truncation error; see equation 2.1, discussed in section 2.3.1. A sufficient accuracy of commercial hydrocodes has to be postulated. ($\rightarrow$ see also "conformity" in section 1.3.2)

3.4.3.5 Consistence

Consistence of time and geometrical discretizations has to be postulated.

Consistence has to be understood with respect to the choice of timestep Δt and element size Δx. The timestep and the element size are dependent to each other. Consistence signifies that for $\Delta t \rightarrow \infty$ and for $\Delta x \rightarrow \infty$ the difference Δ can mathematically expressed by the differential coefficient ∂. In other words the numerical integraton scheme becomes the exact solution of the differential equation and the analytical solution of the mechanical model will be approached.

3.4.3.6 Benchmarks

Benchmarks are an important part of code validation (section 3.3).

By setting up a benchmark problem we can observe that different users achieve quite different results by using different methods and codes. Also different problems occur.

The benchmark tests should be conducted numerically **and** experimentally. But numerical results can not be fitted to experimental results simply by non-physical *curve fitting*. In such a case one cannot learn anything from the numerical simulation.

It has become fashionable to use numerical tools along with the experimental investigation. But sometimes, there exists a confusion about the difference between experimentally determined model parameters (e.g. for the yield curve within the material model) and tuning the numerical input data until the numerical result fits the experimental one.

Thus, it is important to formulate standard benchmark tests against which codes are tested (section 3.3.4).

3.4.4 How to determine the proper timestep

Most hydrocodes use an explicit integration scheme that leads always to problems near boundaries or the axis of revolution because forces and displacements are usually not conjugated like in FE codes. The calculation advances from time t^i to time t^{i+1} without any iterations in between and the differences of the constitutive values are based on the timestep Δt. Because shocks travel distances of millimeters per microsecond (e.g. PETN: $9000\frac{m}{s}$), the timestep must be small enough to resolve the temporal details. To get the right value for the proper timestep, different criteria have to be checked. One of the most important is related to the smallest mesh size Δx and is called COURANT criterion:

$$\Delta t \leq \frac{\Delta x}{c}, \tag{3.2}$$

where c is the soundspeed, which is in case of a shock wave propagation replaced by the velocity of the shock. The wavespeed c is not constant, it changes as the material changes (density, pressure, stiffness):

$$c = \sqrt{\frac{E(\epsilon, \dot{\epsilon})}{\rho(p)}} \quad \text{replaced by} \quad c = \sqrt{\frac{p}{\rho(p)}}. \tag{3.3}$$

The wavespeed c can be identified in the p-ρ-plane: It is proportional to the variable slope of the EoS.

Additionally, the mesh size Δx changes significantly while meshes deform. Thus, the COURANT criterion has to be fulfilled in every timestep.

Eq. 3.2 should ensure that the shock front does not omit a cell. That has been stressed by additionally using a time step correction factor, a so called "safety factor" (< 1), by that the timestep is multiplied. So, no disturbance should be able to propagate across a zone in a single timestep. In case of shock loads, "disturbance" means, for example, the shock width within the mesh.

Shock development

Fig. 3.2 shows the development of a shock that arised from a contact detonation on a concrete plate. The numerical set up and further details are discussed in section 3.5.1.

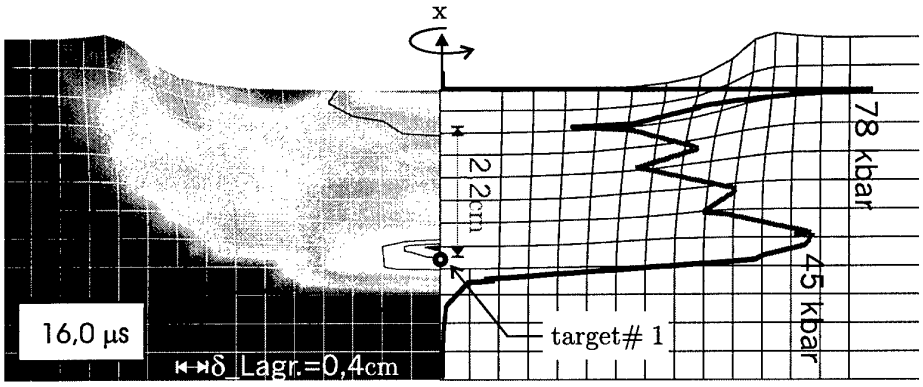


Figure 3.2: Range of shock development (zoom of a crater region)

On the left part of fig. 3.2, the contour-plot of pressure is shown from $p = 0$ to $p = p_{max}$ (here: 78 kbar). On the right part, the distribution of pressure along the axis is plotted.

In [4], BENSON explains that the shock can only sufficiently be treated if it is transfered by approximately four to six elements and the density of the mesh must be fine enough so that *the six element shock width* is small in comparison with the dimensions of the problem.

In the example presented here we have $\frac{2.2cm}{30.0cm} = 7\%$. This aspect can be proved by looking at the range of the shock development which is about $2.2cm$ and includes about six elements (fig. 3.2).

BENSON's demand has, obviously, been satisfied here by using a Lagrange-mesh size of $\leq 4mm$ in the 'critical' zone. Taking into account that the grain size of concrete is up to $32mm$, one could start to argue about the homogenization principle, because the element size is clearly less

than the the grain size.

Proposal:

The COURANT criterion has to be automatically controlled by the code used. In addition, for the sake of reliable and safe numerical simulation of shock waves with hydrocodes, we propose a compliance with BENSON's *six element shock width* demand as a **minimum requirement**.

3.4.5 Numerical treatment of shock oscillations - artificial viscosity

It is a common strategy to smear out the jump discontinuities associated with shocks by special numerical techniques. This is necessary in order to properly handle shocks in a hydrocode simulation. A standard approach is the introduction of an artificial viscosity that has to be incorporated to the governing equations. The role of these terms is to damp out the postshock oscillations (diffusion terms). This is important to obtain physically meaningful solutions.

There exist lots of different expressions for viscosity terms, for example the viscosity formulation by VON NEUMANN & RICHTMEYER from 1950 ([28]). Some of them are described in [4].

The timestep has to decrease as the "diffusion" term, which is related to the artificial viscosity, grows:

$$\Delta t \leq \frac{\Delta x}{A + \sqrt{A^2 + c^2}}; \quad A = 2b_1^2(\Delta x)\left|\frac{\partial v}{\partial x}\right| + b_2 c. \tag{3.4}$$

Herein A and $b_{1,2}$ are numerical parameters that expand the commonly used artificial viscosity term

$$q = \frac{\partial}{\partial x}\left(\mu \frac{\partial v}{\partial x}\right), \tag{3.5}$$

where μ is the common coefficient of viscosity.

In the used code, a linear q-term that provides an additional condition for the timestep

$$\Delta t \leq \frac{\Delta x}{2Bc} \tag{3.6}$$

is included. It contains a linear artificial viscosity coefficient B.

These tools are used for handling shocks by spreading the shock smoothly over several mesh intervals. With this at hand the artificial viscosity q has to be incorporated into the difference equations, e.g. for the pressure p:

$$\partial(p + q)/\partial x. \tag{3.7}$$

The presented pressure history plots (e.g. fig. 3.11) have to be well understood in that manner. Thus, it is evident that difficulties occur especially at the high instantaneous pressures in targets near a detonation.

Proposal:

The influence of artificial viscosity mechanisms should be evaluated. Small variations within those mechanisms must cause small changes in results according to *robustness* that has been postulated in section 3.4.3.2.

3.4.6 The multimaterial Euler processor

Some codes use Euler processors that allow more than one material in a single cell. This multimaterial procedure includes certain rules for mixing the parameters with respect the surface (or volume) fractions of the different materials. But that unavoidably leads to difficulties because some parameters (e.g. the density) are mixed depending on the fractions of the materials in the Euler-cell, whereas other parameters (e.g. the velocity) have to be treated independently from the materials.

This implies that slip is impossible on material interfaces within a multimaterial element. There are no slide lines in these elements. In our special problem (the simulation of contact explosions) the flow of detonation-gases next to the solid body has to be modelled. A boundary layer with a nonzero shear stress occurs in the solid and the velocity profile of the gas is altered because of the "artificial sticking condition" within mixed elements (BENSON [4]).

Proposal:

One should be aware of problems concerning the multimaterial processor. Corrective measures are mesh refinements which might reduce these problems.

3.4.7 Treating distorted cells

The mesh distortion in the Lagrange-mesh during a simulation of a contact detonation is shown in fig. 3.3, where the region nearby the crater has been zoomed out.

It is evident that numerical results might not be trustworthy if large distortions occur. In numerical simulations one has to take care that the quadrilateral elements cannot be distorted into "boomerangs" or "bowties", as shown in fig. 3.4.

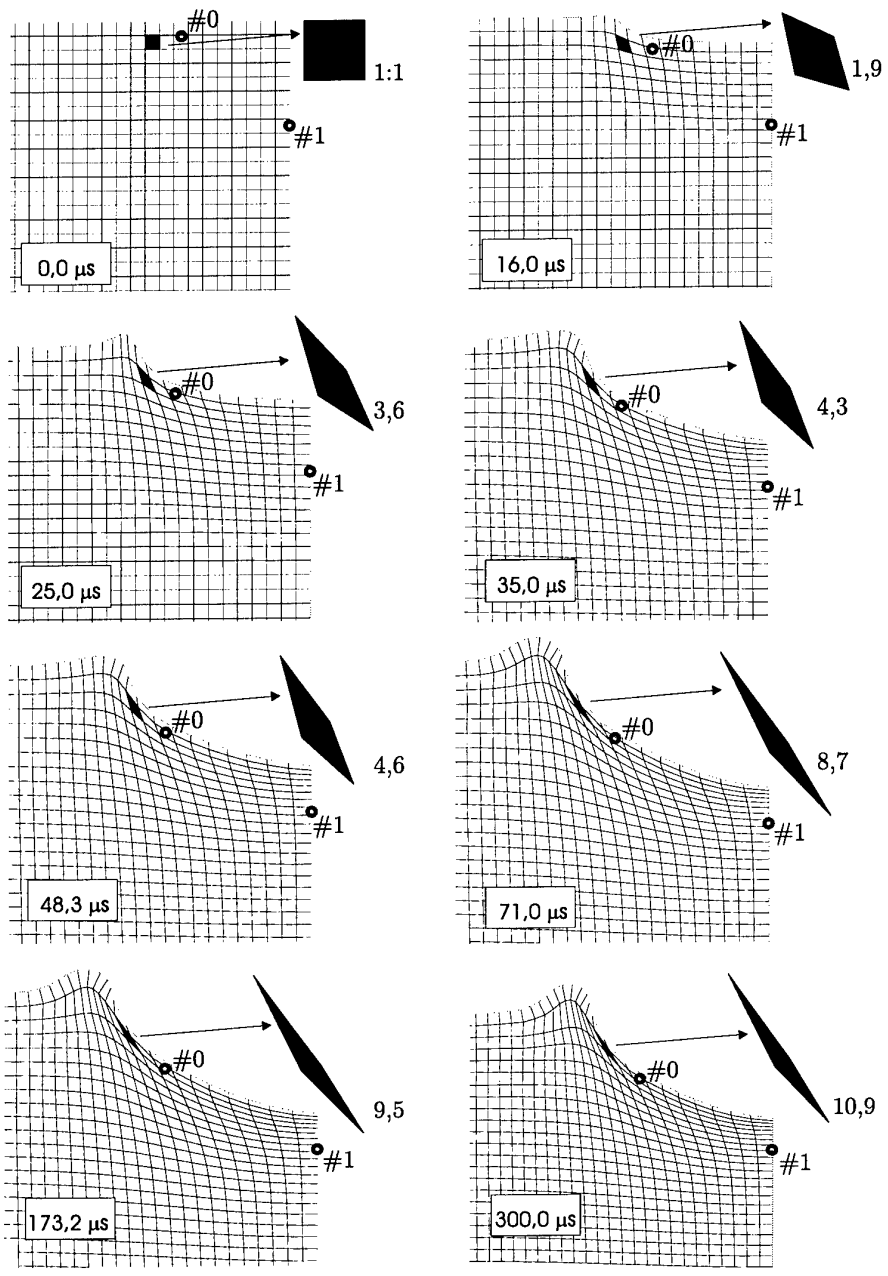


Figure 3.3: Distortion of Lagrange-elements nearby the crater

If the timestep is small enough and the strains are not too large, it is impossible to push a node of a cell into its opposite edge because the numerical volume then approaches zero, leading to an infinite residual pressure. The numerical integration scheme is only exact on the master element which is a square. The more distorted, the poorer the result.

A big problem of self- or adaptive meshing is that elements might be already distorted in the initial unloaded situation. We don't use self- or adaptive meshing here.

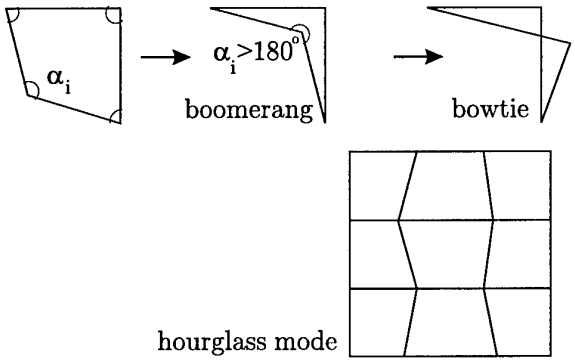


Figure 3.4: Large mesh-distortion and hourglassing

The distortion of elements can be controlled by different strategies:

1. The inner angle α_i between edges has to be $< 180^o$.
2. The determinant of the Jacobian Matrix is not allowed to become negative, otherwise $dV = det(J)\ dr\ ds\ dt$ yields negative numerical volume.
3. The change in ratio of diagonals (1:1 for the quadratic master element), see fig. 3.3

Using "constant stress quadrilateral elements", might cause zero energy modes. This is called hourglassing (fig. 3.4). To ensure that no hourglassing occurs, certain control-algorithms have been included in the most commercial codes.

About damping algorithms

Handling hourglassing by special tools is one specific example for a damping algorithm. There might also be others, like smoothing peak pressures. Such algorithms shuold be treated very carefully. For a detailed insight we refer to BENSON [4].

3.4.8 Conclusion

Section 3.4 has given insight into the basics of hydrocodes. Some typical problems have been revealed, and demands and proposals have been stated, for the purposes of a quality improvement of hydrocode simulations.

Nevertheless, the generally stated demands and proposals have to be well targeted to the special problem that has to be solved by the user.

To illustrate and deepen the background given in this section, two specific hyper dynamic problems are exemplarily selected and discussed in the following *reliability study* (section 3.5):

- Contact detonation (section 3.5.1),
- penetration and perforation (section 3.5.2).

3.5 Reliability study

The following examples are *own numerical simulations* with AUTODYN concerning reliability and safety. Special focus is done on *asymptotic convergence* that has been well defined in section 3.4.3.1.

3.5.1 Example 1: Contact detonation

3.5.1.1 Load level regions

Explosive charges cause various regions of stress and failure situations, as shown in fig. 3.5.

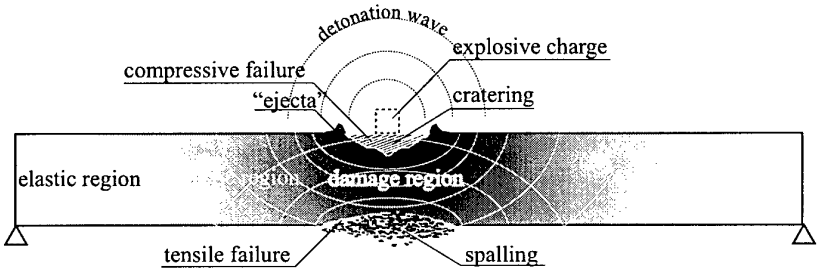


Figure 3.5: Contact detonation on a concrete plate, regions of different stress states and failure situations

As a result of the detonation, regional limited material failure can be observed. At the top surface of the plate, the concrete material mainly fails due to high compression. This crushing causes a crater. At the opposite side, the shock wave is reflected and converted into a tension wave. Because of the low resistance of concrete to tension, one can observe a tensile spalling. Between these regions there is a part where concrete suffers certain levels of damage.

3.5.1.2 Numerical set up

Fig. 3.6 shows the numerical set up for the Hydrocode AUTODYN2D. Because of the problem we can take advantage of the axial symmetry. The explosive charge of 650g TNT (numerically described by the well-known JONES-WILKINS-LEE equation) is centered on a circular-plate made of unreinforced concrete. The charge is in contact with the concrete surface.

The Eulerian mesh wherein air and expanding detonation gases (material without strength) are simulated is coupled with the Lagrangian mesh that enables the modeling of the solid (material with strength) structure. This requires an overlapping of these two meshes. The choosen overlapping (here 10cm) has to ensure that the crater-region of the deforming Lagrange-mesh

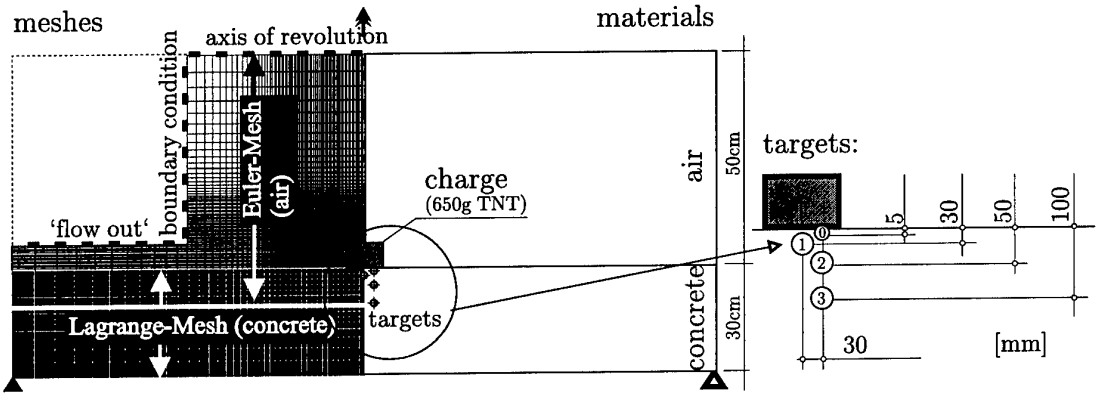


Figure 3.6: Numerical simulation of a contact explosion on a concrete plate

is sufficiently overlapped by the Euler-mesh at any time. Therefore, the proper overlapping measure can only be found with the help of a pre-study.

In order to prove asymptotic convergence (section 3.4.3.1) and to quantify remaining errors the problem set up, which is given in fig. 3.5 and 3.6, is examined.

3.5.1.3 How to choose characteristic parameters

Applying displacement formulated finite elements, displacements converge even better than their derivatives, e.g. strains. Because the stresses are directly related to the strains by constitutive laws for the material, the convergence of stresses or strains, respectively, must be proved. In this case we can state:

Asymptotic convergence of the displacements is only a necessary condition, the convergence of strains (stresses) is a necessary and sufficient condition.

Or more general: *Asymptotic convergence has to be carried out with respect to the parameters of the governing equations (characteristic parameters), that include the highest order of the derivative of the given problem.*

The parameters given in the governing equations for hydrocodes (eq. 3.1) are pressure, volumetric strain (or density) and internal energy (or enthalpy) ([1], [3], [4]). These are parameters on the lowest level of the formulated constitutive equations if macromechanics is adopted. So, these parameters are *characteristic parameters* to be chosen for convergence studies. Consequently, the proof of their convergence is necessary and sufficient. The proof of convergence of integrated values, e.g. impulse, is only a necessary condition.

Doing so, the convergence studies here are carried out with respect to the parameter "pressure

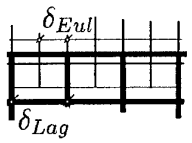
p" (figs. 3.8 and 3.10) which is calculated from stresses.

3.5.1.4 Euler-Lagrange mesh-ratio

The Euler-Lagrange coupling algorithm provides a simultaneous use of both processors in one numerical simulation (e.g. [3], [12]). The proper interaction of the Euler mesh and the Lagrange mesh depends - among other things - on the Euler-Lagrange mesh-ratio.

A detailed mesh-ratio study has been done by the authors in [20]. The results are resumed in this section.

The columns in fig. 3.8 represent the maximum pressure '**P**' versus the $\delta_{Lag.}/\delta_{Eul.}$-ratio, where $\delta_{Lag.}$ is the Lagrangian and $\delta_{Eul.}$ is the Eulerian mesh size. Ratio 2, for example, means that there are twice as much Euler-elements than Langrange-elements with respect to the edges (fig. 3.7).



$$\triangleq \quad \frac{\delta_{Lagr.}}{\delta_{Euler}} = \frac{2}{1}$$

Figure 3.7: Example: Lagrange-Euler-Ratio = 2:1

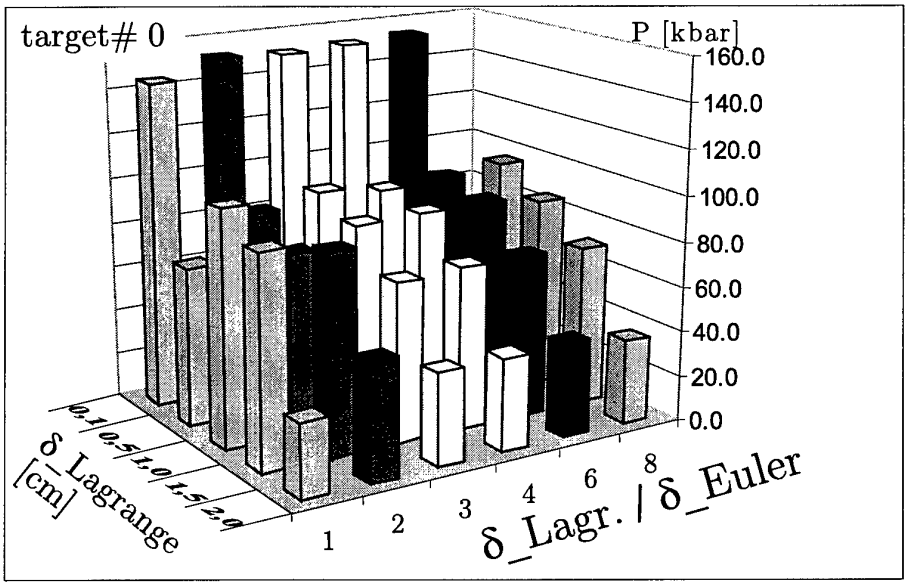


Figure 3.8: Maximum pressure vs. mesh sizes and $\delta_{Lag.}/\delta_{Eul.}$-ratio in target #0 (figs. 3.6 and 3.9)

One result from the study displayed in fig. 3.8 is that the ratio between the both mesh types

should be as follows:

$$\frac{\delta_{Lagr.}}{\delta_{Euler}} > \frac{2}{1}. \tag{3.8}$$

From fig. 3.8 one can see that - with respect to the suggested restriction (eq. 3.8) - the quality of the result is almost independent of the mesh-ratio if eq. 3.8 is fulfilled. Fig. 3.8 also reveals an increase of peak pressure when refining the mesh. This is in contradiction to the convergence theorem (section 3.4.3.1), and - obviously - in fig. 3.8 asymptotic convergence cannot be observed. This will be explained in section 3.5.1.5.

Because of the tremendeous rise of calculation time with increasing number of cells, a ratio of 2 (as shown in fig. 3.7) has been choosen for our elementation (pre-)study. Conducting the same study with a ratio of 3 would multiply the calculation time with a factor of > 3, whereas the significance of the result concernig elementation would be the same.

Proposal:

For the simulation of contact detonation problems using Euler-Lagrange coupling, a ratio between 2 and 4 is best with respect to both, proper exchange of data (pressure, particle velocity, displacements between the two different mesh types) and lowest expense of calculation time.

According to the robustness criterion (section 3.4.3.2), we propose a ratio of $\frac{\delta(Lagrange)}{\delta(Euler)} = 3 \pm \partial$, where ∂ should be about 10% of the Euler element-size [32].

3.5.1.5 How to Choose Target Points

Based on the physics, the structure which is numerically simulated should properly respond everywhere. Due to the convergence theorem (section 3.4.3.1) one would expect convergence everywhere, in general. That this might not be the case is illustrated in this section. The study is based on the problem given in figs. 3.5 and 3.6. We also refer to what has been mentioned in section 3.5.1.4.

Fig. 3.9 highlights the target points, already given in fig. 3.6.

We recall fig. 3.8 which data correspond to target #0, that it is directly nearby the contact detonation. Here the methodical inherent problem in determining the discretization error becomes clear: No asymptotic convergence can be observed in target #0.

In fig. 3.10 the results of three target points have been compared, with respect to the fineness of the mesh. We could not reach asymptotic convergence in targets #0 and #1. Only beginning with target# 2 asymptotic convergence could be proved. Several studies with hydrocodes led

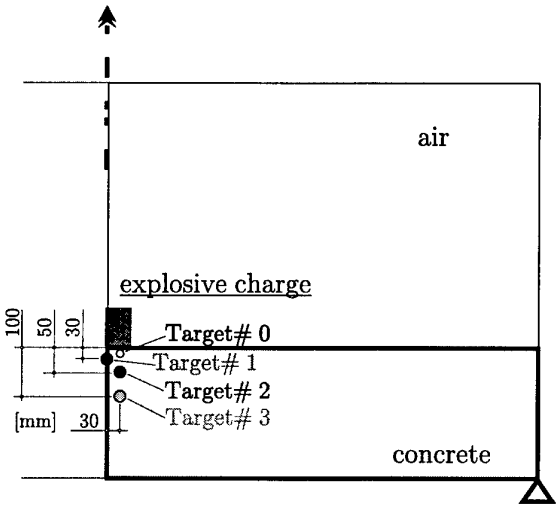


Figure 3.9: Target points

to the answer that one cannot expect convergence at targets nearby the range of instantaneous shock development. The reasons are described in section 3.4 and that is not specific for the used code only.

Convergence can be expected if the target points are out of a nearby region around the contact charge. Very close to the explosive charge convergence is not guaranteed.

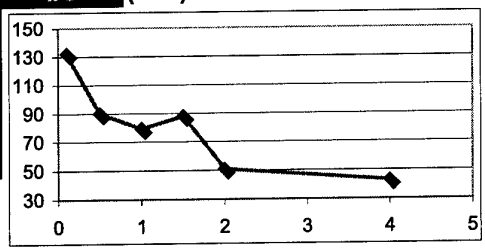
Fig. 3.11 shows the time plot of the pressures with respect to different meshes. The pressure-time plots correspond to target #1. One can see the different peaks and shapes of the pressure-time plots with respect to different mesh sizes. The mesh size varies here from 3.0 to 0.5 mm in the Euler grid. The Lagrangian grid is twice the size, as mentioned before (it runs from 6.0 to 1.0 mm).

3.5.1.6 Resume

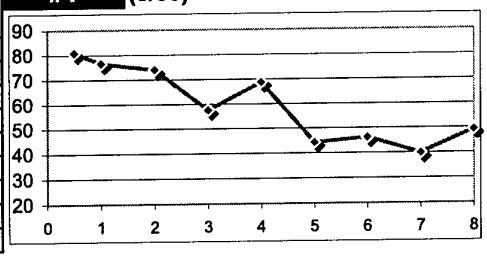
The greater the distance of the target points from the contact charge, the better the asymptotic convergence of pressure-time plots. But in order to sufficiently compute the stress state in the material, it is necessary to ensure convergence in all possible regions even as close as possible to the contact charge. If convergence has not been proved, one does not know how far away the numerical solution is from the exact solution.

In case of nearby-detonations, when there is no contact between charge and structure, hydrocodes reproduce the experimental facts qualitatively and quantitatively in all regions of the structure, but not in case of contact detonations. Therefore, the target points should be located where the

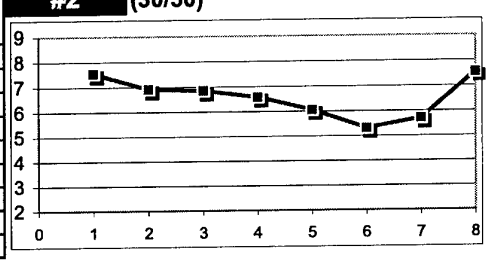
δ_Euler [mm]	pressure [kbar]
0,1	132,0
0,5	90,0
1	79,2
1,5	88,0
2	51,0
4	43,0



δ_Euler [mm]	pressure [kbar]
0,5	80,8
1	76,5
2	74,0
3	57,6
4	68,8
5	44,3
6	46,3
7	40,0
8	49,3



δ_Euler [mm]	pressure [kbar]
0,5	
1	7,5
2	6,9
3	6,9
4	6,6
5	6,1
6	5,3
7	5,7
8	7,5



δ_Euler [mm]	pressure [kbar]
0,5	
1	1,77
2	1,72
3	1,87
4	1,83
5	1,54
6	1,57
7	1,39
8	1,18

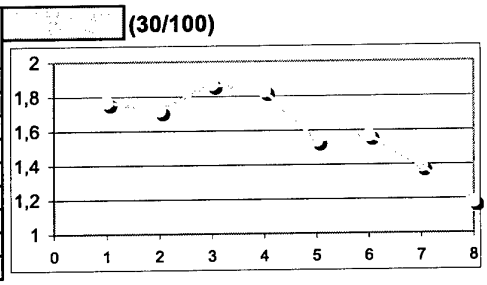


Figure 3.10: Peak Pressure vs. mesh fineness for different targets

elements remain almost undistorted, where the strain rates are moderate ($\leq 10^4 \frac{1}{s}$) and where the shock wave velocity is in the range of the soundspeed.

Of course, the pressure peaks and the stress peaks, respectively, are the most sensitive values, whereas the impulse converges faster, because it is an integrated value. But it is a wrong conclusion from this to choose the impulse as characteristic parameter for asymptotic convergence studies. The impulse is not a parameter in the constitutive equations.

It would be very useful to rezone and/or to refine the Lagrangian mesh if it becomes significantly

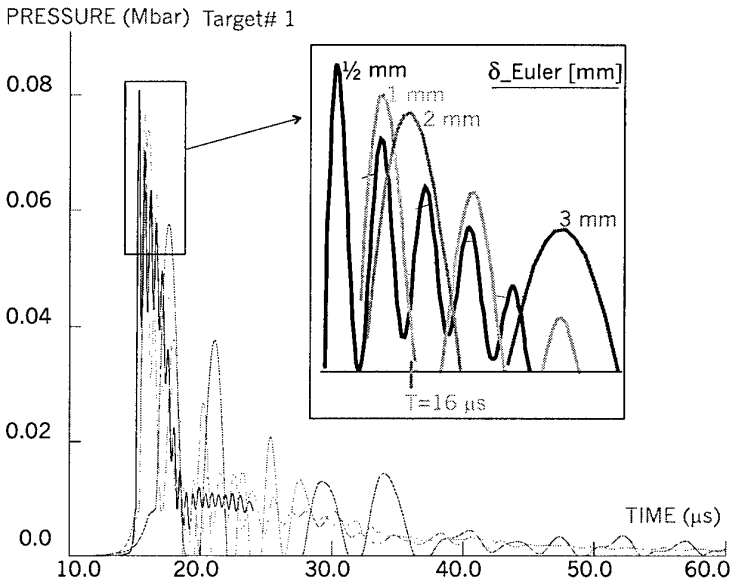


Figure 3.11: Pressure vs. time for different mesh sizes for target# 1

distorted. But, the user has to pay by increasing computation time. In addition, it is not an easy task to obtain a clear declaration about the convergence from the momentum-time plot. The time-integration of pressure is unfortunately not unique. The integration limits are not easily choosen because of the fact that the pressure intersects the time axis somewhere, but not at the same time for every mesh size. To choose a specific time limit for the integration of the pressure, produces no declaration about convergence as well, because the momentum would not be unique by this.

The momentum that is derived by the integration of the pressure with respect to time is shown in fig. 3.12.

The only possible statement is that at critical target points (#0 and #1) the momentum does not asymptotically converge to a certain reference momentum-time curve.

Conclusion:

The conclusion taken from these studies is that one can not expect convergence in a *critical region* around the contact detonation. In the presented case of a specific contact detonation, the boundary of this region is of about 3 cm (8 elements) around the contact surface. Inside of this zone the numerical results are not reliable (fig. 3.13).

But where are the reasons for this?

A pre-study only with air that is modelled by an ideal gas Equation of State (without any

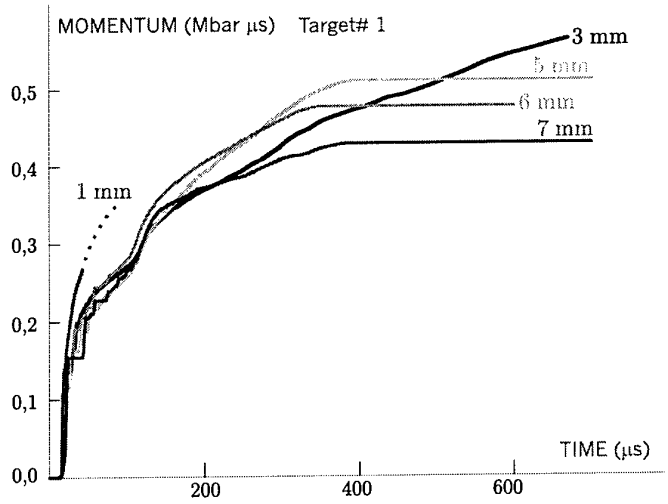


Figure 3.12: Momentum vs. time for different mesh sizes

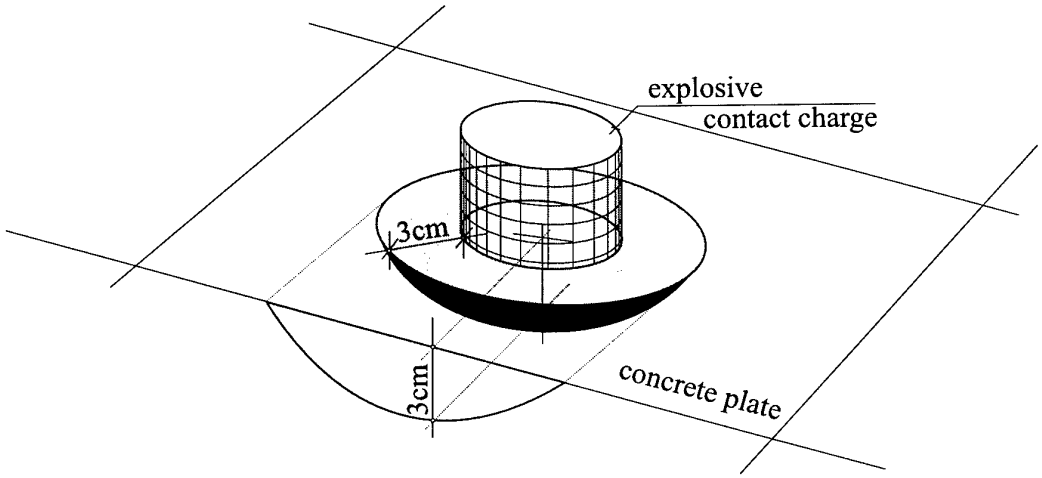


Figure 3.13: The "critical" region around the contact detonation

additional constitutive laws) has been carried out. In a limited region within an Euler-mesh, the initial specific internal energy has been modified so that initial pressures similar to an explosion have been approached. Doning so, neither contact nor coupling of Euler- and Lagrange-grids was necessary. Even in that simple case, convergence problems concerning pressure nearby the high-pressure-zone have occured [32].

But at our special research subject of contact explosions on concrete additional problems occur. So, one should have deep knowledge and a right feel for all the problems that occur especially at the overlapping zone. The problems are:

- the coupling of Euler and Lagrange (overlapping) especially the exchange of informations,

- the nonlinearity in constitutive laws,
- large Lagrange-element distortions,
- the nonlinearity of deformation,
- extremely high pressures and rates,
- a constant stress assumption similar to a single point integration.

If the interaction between load and structure has to be considered, the coupling of Euler and Lagrange meshes is enforced. If in addition the load is shock-like, problems in the overlapping zone occur. In section 3.4 some methodical inherent problems are briefly discussed in order to well understand the reasons.

3.5.2 Example 2: Penetration and perforation

3.5.2.1 On the numerical set up

A concrete plate is impacted by a steel-copper-projectile. The numerical set up is shown in figure 3.14.

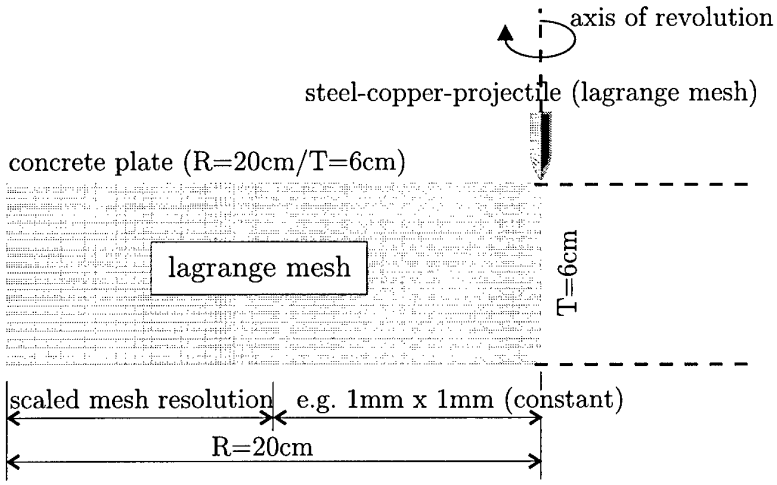


Figure 3.14: Numerical setup of a penetration-perforation study

Here we use the hydrocode AUTODYN2D and the developed concrete model by RUPPERT ([32], [22]). The projectile has got a steel kernel and a copper liner. The tip has got an ogive kind of shape. For details we refer to [32].

Focus on the projectile

The tip has been meshed by joining the nose part and the body part (fig. 3.15). The given projectile dimensions are $8 \cdot 26$ [mm].

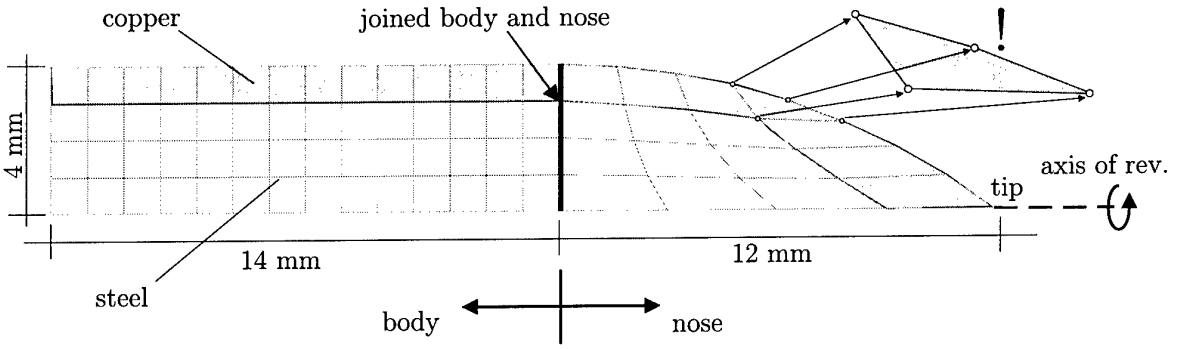


Figure 3.15: Projectile elementation

Figure 3.15 shows the elementation of the projectile. One specific cell of the nose has been zoomed out. This element is inadequate and might cause numerical difficulties due to the lagrange mesh deformations (section 3.4.7).

We run the risk that this element might be distorted into a boomerang or into a bowtie. Thus, also an alternative meshing method for the projectile nose has been adopted as shown in fig. 3.16.

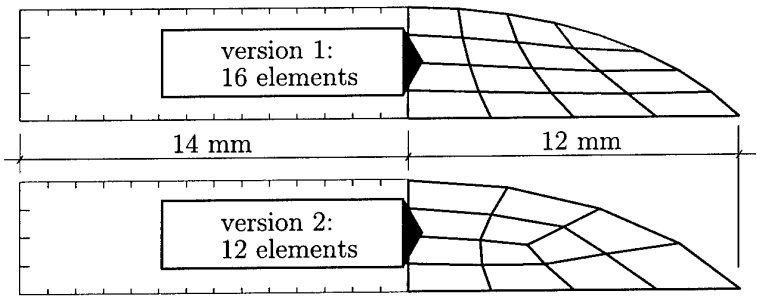


Figure 3.16: Meshing: Two versions for the projectile nose meshing

Conclusion

The evaluation of exit velocities of the projectile for the two different projectile meshes is shown in figure 3.17. Version 2 has got no "problem cells".

The results (concerning the exit velocity) are similar but differences are observable. But the results differ relatively small and they are obviously based on the difference of mesh fineness

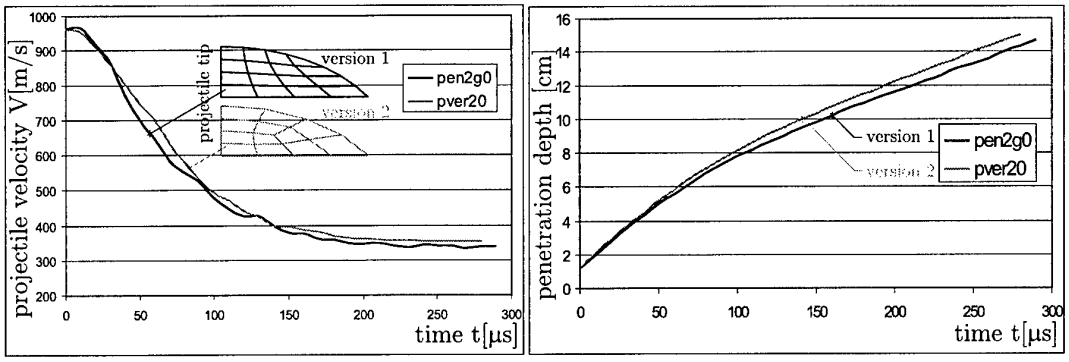


Figure 3.17: V-t and s-t-diagram

(mesh resolution) between the two elementations: Version 1 has got 16 elements; version 2 has got 12 elements.

Nevertheless, we propose to use version 2 for further penetration/perforation studies, because mesh distortion problems cannot occur at least at the beginning of the calculation.

In the following section the inflence of the mesh resolution for the concrete plate will be shown briefly.

3.5.2.2 Convergence

As mentioned above in detail (section 3.4.3.1), the elementation (mesh density, ...) might significantly influence the numerical results. To draw conclusions also in the field of penetration and perforation, a mesh density study has been conducted (see RUPPERT [32]) and the results are shown here.

It is important to determine the appropriate mesh densities and to find an optimum mesh ratio if possible, in order to fulfill the convergence theorem (section 3.4.3.1).

For this convergence study, a concrete plate with $T = 6$cm of thickness has been choosen. The projectile (metal inside and copper shell) has got an initial velocity of $v_0 = 455\frac{m}{s}$. Experimental investigations have not been carried out here.

The results are evaluated by space-time-diagrams with respect to the exit velocity, that increases with mesh density (fig. 3.18).

As shown in figure 3.18 asymptotic convergence can be achieved: The exit velocity is not significantly increasing by refining the (concrete-)mesh from 1mm to 0.5mm and again to 0.25mm. A further mesh refining will not significantly change v_{exit}.

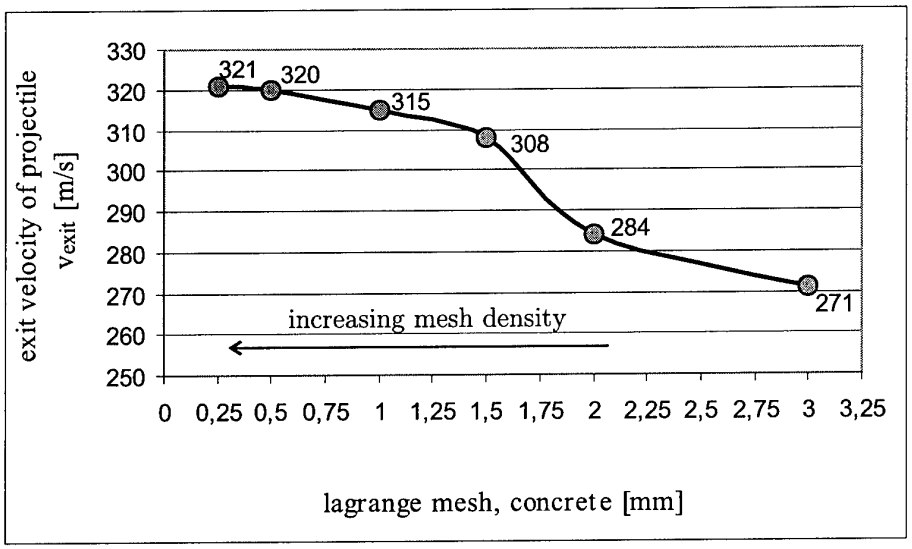


Figure 3.18: Asymptotic convergence of the exit velocity for increasing mesh density, for $v_0 = 455\frac{m}{s}$

3.5.2.3 Influences of internal parameters

According to the algorithm applied, internal parameters govern the numerical calculation. Penetration/perforation problems are usually solved by a Lagrange-Lagrange coupling algorithm (e.g. BENSON [3]). Thus, we focus on internal Lagrange-Lagrange interaction parameters here. A summary of our penetration/perforation study is briefly shown in this section and the most important internal parameters have been evaluated (taken and modified from RUPPERT [32]).

The relevant interaction parameters that have to be specified, are:

- **Gap size and gap algorithm**: Numerical methods based on FE discretization don't work when cells are overlapping or penetrate into each other (section 3.4.7). In consequence of the Lagrange-Lagrange coupling algorithm, the involved Lagrange meshes must have a certain distance to each other in order to avoid cell overlapping. Therefore, a gap size has to be well specified. This gap is not physically, it is just a numerical feature! It can be modelled geometrically (visible gap) or it can be represented invisible (internal gap) [12].

- **Friction**: Friction between materials at the slide-line of their meshes can be considered by a specific coefficient of friciton. Friction might also be neglected in certain circumstances depending on the problem to be solved.

- **Time step**: How to determine the proper time step is crucial for explicit codes (section

3.4.4). The time step is multiplied by a specific safety factor (< 1). This prevents overlapping of opposite cells, because by this feature it is impossible to overjump the gap in one single time step.

- **Erosion**: Erosion is a special feature to transform elements into free mass points by an user specified erosion criterion. This technique might be powerful to handle distorted cells that are caused by deep penetrations and perforations [12]. For example: If a specific *effective plastic strain* ϵ_{eff}^{pl} is exceeded, the relevant cell will be eroded. In our problem this signifies that the protectile's outer layers are stripped off during the penetration into a concrete plate.

- **Inertia**: The user has got the possibility to swich on or to swich off mass inertia effects of the eroded cells (if erosion is used). We observed that the erosion criterion is mesh sensitive. Thus, erosoin and inertia of eroded cells have to be used carefully [32] and we prefere a detaild pre-study when using these numerical features.

The variation of internal parameters from the default values by the user might cause changes of the numerical results. It is the user's duty to **validate** their influences. Therefore, primarily the **robustness** has to be checked (section 3.4.3.2).

Our Lagrange/Lagrange-interaction study reveals the influences of the most important internal parameters, qualitatively as well as quantitatively. The results are shown in tab. 3.2 where the projectile's exit velocity V_{exit} is the observed parameter.

Table 3.2: Influences of internal Lagrange/Lagrange parameters

Internal interaction parameter	"default" (AUTODYN2D)	Variation done	this influences V_{exit}
Gap size [mm]	0,20	(0,08) 0,13 - 0,25	(30%) 4%
Gap algorithm	visible	internal	25%
Friction	off	on: 0,02 - 0,08	observable, but remote
Time step (safety factor)	β=0,2	0,1 - 0,2	observable, but remote
Erosion (projectile)	off	ϵ_{eff}^{pl}=200%	27%
Inertia of eroded cells	off	on	25(!)%

It becomes evident, that specific internal parameters influence the results. For example, the inclusion/exclusion of the inertia of eroded cells or the value of the numerical gap size are significantly changing the projectile's exit velocity. Up to here, none material parameter has been discussed.

Nevertheless, **all the variations done here are within the limits suggested by the tool's manuals!**

Conclusion:

Without this study no substantial statement can be made upon the choice of internal interaction parameters within the Lagrange/Lagrange-interaction algorithm. Thus, we recommend not to just trust on the defaults.
And the question comes up: "Are **all** internal parameters accessible and changeable by the user?" Of course this is just a rhetorical question and some of the **interaction parameters are hidden behind the "black box"**. The influences of all internal parameters will not appear to the user unless the code developers let him know the "secrets". But for the purpose of *quality assurance* of numerical simulations, we attach importance to the *traceability* of all internal parameters used in the codes.

3.5.2.4 Remarks

Although this study on v_{exit} is important to do, it is not a complete and sufficient convergence study for penetration and perforation phenomena at all. The asymptotic convergence of the exit velocity is only a necessary but not a sufficient condition.

Thus strictly speaking, a sufficient fulfillment of convergence implies the asymptotic convergence of the methodical inherent state variables within the conservation equations.

Hyperdynamic problems solved by the authors

In [32] some numerical studies are given with the following topics:

- Free and near field detonation,
- indoor explosions +interaction with structure,
- contact detonation,
- bodies' impact, penetration and
- perforation

Chapter 4

Proposal to develop user guidelines

One never can stop learning, if one wants to keep up with the time. This *law* becomes obvious particularly with regard to using numerical methods and tools. This chapter focuses on the user. Every user is livelong a trainee; the assistant or person in charge who executes an application and the scientific user who develops the numerical tool as well as the person who must be able to assess and evaluate the results.

4.1 Intention

The intention is to accompany the user for the sake of a credible use of finite methods by user guidelines. The theoretical background has been supplied before (chapter 3). This chapter outlines the basics to develop individual and managable user guidelines for specific hyperdynamic problems.

4.2 The cycle in general

In the following focal points that have been mentioned above and that are relevant for the user are sumarized here:

- The task
- Description of reality
- Mechanical model
- The method

- The tool
- Handling results

Our conception has to be understood as a **checklist** that accompanies the user from the first step, *understandig the task* to the final step: *handling the results.*

We use the term *"cycle"*, because this schedule has not to be treated just by the top-down method beginning from the first topic ("The task") and ending at the final topic ("Handling results"). Rather, the user might continually jump between the topics back and forth. For example, the topic "The tool" can not handled seperately from the method on wich the tool is based on. Also the topic "Mechanical model" can not be ticked off when results of the numerical simulation are discussed; changing the mechanical model and afterwards starting the calculation again might often be advantageous. Scrutinizing the results will often force the user to go the upper topics.

Of course, the items have to be individually arranged and adjusted to the specific task that has to be solved by the user. Thus, this list is certainly not comleted. Depending on the task, some items listet in the following are unnecessary. Therefore, it's on the user to make his individual checklist before starting to solve his specific problem.

4.3 Checklist

Task

- Get deep insight: Comprehension of the problem to be solved
- → What is the goal of the study?
- List all *interested parties* and their relations (section 1.3.4, fig. 1.1)
- Classification of the task (section 1.4.1):
  - Loading situations and loading rates,
  - Structural behavior / local behavior (section 1.4.3)
  - Total distortions
  - Peak pressures (estimation)
- Survey and research:
  - Have similar tasks already been solved?
  - Are test results available?
- Evaluation/estimation of the task:
  - Application of resources: Personnel (user(s)), tools (software) · time
  - Is additionally external expertise advantageous?

Description of reality

- Geometry
- Motions
- Materials
- Loading situations
- Boundary conditions
- Symmetries
- Extent (spatial and temporal)
- Other environmental conditions

Mechanical model

- Plot all specific key parameters in a list:
  - Geometry: Extentions, dimension (2d/3d), symmetry, spatial restrictions
  - Structural components: Rods, plates, springs, damping devices, connections
  - Boundaries: Constraints and supports, environmental conditions, flow out of materials

  - Loadings: Applying, temporal process, loading combinations
  - Materials: Constitutive equations, specific material laws
  - Interactions: Describe the contact of components (friction, rigid interfaces, ...)
- Simplifications:
  - Description: List all simplifications done
  - Discussion: Evaluate the influences of simplifications
- Consider a couple of possible mechanical models, not only one
- *see also section 2.2*

Method

- What methods are alternatively available?
  - Element Methods:
    - FDM: Finite Difference Method
    - FEM: Finite Element Method
    - BEM: Boundary Element Method
  - Meshless Methods:
    - SPH: Smoothed Particle Hydrodynamics
    - EFG: Element-Free Galerkin
    - (and others)
- What ist the best method? (section 2.3.5)
- Time discretization:
  - Explicit or implicit integration?
  - Time step pre-restriction: min., max., +safety factor
  - Time step regulation in the explicit integration scheme
- *see also section 2.3*

Numerical modeling

- Transfer the parameters of the mechanical model into the code (section 2.2):
  - Are further restrictions and simplifications necessary?
  - Which additional (numerical) parameters are introduced?
    - Choice of a consistent unit-system
    - (...)
  - Transfer to the software; see **"Tool"**: Preprocessing algorithm
- Spatial discretization:
  - Choice of elements: Triangle, quadrilateral, element functions
  - Definition of wrapup criteria

  - Are further pre-restriction necessary?
  - Are boundary conditions changing during the simulation?

- Specific items:
  - Internal truncation error and numerical stability (sections 2.3.4.2, 3.4.3.3, 3.4.3.4)
  - Handling shock oscillations: Artificial viscosity (section 3.4.5)
  - Treating the multimaterial (Euler-)processor (section 3.4.6)
  - Euler-Lagrange coupling, Lagrange-Lagrange interaction (sections 3.5.1, 3.5.2)
  - Treatment of distorted elements: Handling hourglassing, avoid bow tie (section 3.4.7)
  - Return algorithm: According to associated or nonassociated flow
  - Damping algorithms
  - Fluid transport algorithm
  - Stress computation: e.g. a constant stress asumption within a single cell (section 2.3.4.3)
- Definition of wrapup criteria:
  - Temporal: Time step
  - Spatial: Smallest element size
  - Internal: Int. energy vs. reference energy
  - Stress (pressure)
  - Cutoffs:
    * Velocity
    * Boundary conditions: e.g. flow criteria
    * and possibly others
- Contact algorithms:
  - Interaction procedure: e.g. penalty algorithms, gap, exchange of state variables
  - Formulation of friction: rate dependency?
- Point out all sources of errors; see section 2.3.
- (see also chapter 3)

Tool

- What tools are available? (section 3.1.1)
- Limits of applicability and accordance with the methods?
- Are independent calculations possible/necessary?
- $\rightarrow$ choice of the best tool according to the best method.
- What is provided by the tool and
- assumed to be axiomatic right? (for example the JWL-EoS for explosives!)
- Input check:

  - (The handling the tool according to the preprocessor should be "ticked off")
  - Take care on consistent unit systems and on
  - the material-fill method

- Integrity check:
  - Are all items available within the tool, that have been mentioned at the topic *"The method"*?
    * If so:
      · How are this items transfered to and integrated into the tool used?
      · Are the concerning parameters changeable/variable by the user?
    * If not so, initiate further steps:
      · Go through the manuals in detail, research and/or
      · ask the software developers for more information

- First step; approach the problem by small pre-calculations:
  - Define small and handable tasks as extracts of the whole problem
  - (...)

- Further step; benchmarking (sections 3.3, 3.4.3.6):
  - Benchmarking against test results
  - Benchmarking against different tools

- Next step; controlling:
  - to what extent can the results be transfered from the first step and from benchmarking to the specific problem?
  - Region of divergence? Is the convergence theorem satisfied? (sections 3.4.3.1, 3.5)
  - Conduct the "first step of code validation" (section 3.3.3)
  - check BENSON's demand (section 3.4.4)
  - modify all specific parameters:
    * validate (weight) the parameters
    * check robustness of all governing parameters
    * check robustness of all internal parameters
    * (for *robustness* see also section 3.4.3)

- Final step; simulation of the task:
  - Not only with one single tool
  - Not only by one single (by the same) person
  - Not only one single mechanical model
  - Conduct a simplificated 2d-simulation and compare to 3d

- $\hookleftarrow$ *Modificate and start again from "Mechanical model"*

Handling results

- Post-processing and visualization of results (section 3.2):
  - Possible plots are:
    * displaced shape plots,
    * contour plots of displacements,
    * plots showing reaction forces and moments,
    * listing of stresses or strains sorted by ascending or descending magnitude,
    * contour plots of stresses or strains,
    * vector plots showing the directions of principal stresses,
    * plots of stresses or strains along paths,
    * plots of deflection, stress or strain against time,
    * path integrals such as J-integrals for fracture mechanics.
    * Multiplots: Mixed plots of all above
  - Take care of the following:
    * Plot results not only at the end of a calculation
    * Where is the exact position of the target points?
    * Are the target points fixed or (Lagrange-)cell related moving?
    * Switch on/off the posprocessor's smooth algorithms
- Comparison to analytical results (if possible)
- Comparison to experimental results (see *benchmarking*)

(...)

4.4 Integration into a quality management system

According to the checklist above (section 4.3), the user has to design a suited and individual checklist concerning his special problem to be solved. A critical evaluation of all the listed items has to point out crucial points. This individual (modified) checklist leads to a **specific user guideline**.

It can also be understood as a **quality manual document**, that describes the total process in detail and states results achieved, or that provides evidence of activities performed.

For the sake of an objective evidence (section 1.3.2), this quality manual might be accredited by an accreditation council (section 1.3.3). The main characteristics of this council have to be independence, objectivity and high quality. The agency has to be oriented towards the realization of both, academic principles and practical usage, e.g. for a proper code validaton and benchmarking (section 3.3). It has to be neither influenced by any states, governments, interest groups nor by lobbyists. Like a scientific institute at the university, academic freedom and autonomy have to be respected: They may regulate their own quality and standards, but at the same time they must guarantee transparency of process and public accountability in discharging this self-regulation.

The central goal is to provide transparency as well as to meet all the requirements. By this at hand, maintenance and enhancement of quality of numerical results is supported. A parallel objective is to provide guidance and information for beginners (e.g. students), code users, code developers and also scientific institutions.

Declarations

****

(1) In accordance with Defense Federal Acquisition Regulation 252.227-7036, Declaration of Technical Data Conformity (Jan 1997), *All technical data delivered under this contract shall be accompanied by the following written declaration.*

"The Contractor, University of the Bundeswehr, hereby declares that, to the best of its knowledge and beliefe, the technical data delivered herewith under Contract No. F61775-00-WE051 is complete, accurate, and complies with all requirements of the contract."

DATE: 11/26/07
Name and Title of Authorized Official:

(2) In accordance with the requirements in Federal Aquisition Regulation 52.227-13, Patent Rights–Aquisition by the U.S. Government (Jun 1989), *CONTRACTOR WILL INCLUDE IN THE FINAL REPORT ONE OF THE FOLLOWING STATEMENTS.*

( ) "Disclosures of all sibject inventions as defined in FAR 52.227-13 have been reported in accordance with this clause."

(X) "I certify that there were no subject inventions to declare as defined in FAR 52.227-13, during the performance of this contract."

DATE: 11/26/07
Name and Title of Authorized Official:

****

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